Abstract

The randomness in Stochastic Gradient Descent (SGD) is considered to play a central role in the observed strong generalization capability of deep learning. In this work, we re-interpret the stochastic gradient of vanilla SGD as a matrix-vector product of the matrix of gradients and a random noise vector (namely multiplicative noise, M-Noise). Comparing to the existing theory that explains SGD using additive noise, the M-Noise helps establish a general case of SGD, namely Multiplicative SGD (M-SGD). The advantage of M-SGD is that it decouples noise from parameters, providing clear insights at the inherent randomness in SGD. Our analysis shows that 1) the M-SGD family, including the vanilla SGD, can be viewed as an minimizer with a data-dependent regularizer resemble of Rademacher complexity, which contributes to the implicit bias of M-SGD; 2) M-SGD holds a strong convergence to a continuous stochastic differential equation under the Gaussian noise assumption, ensuring the path-wise closeness of the discrete and continuous dynamics. For applications, based on M-SGD we design a fast algorithm to inject noise of different types (e.g., Gaussian and Bernoulli) into gradient descent. Based on the algorithm, we further demonstrate that M-SGD can approximate SGD with various noise types and recover the generalization performance, which reveals the potential of M-SGD to solve practical deep learning problems, e.g., large batch training with strong generalization performance. We have validated our observations on multiple practical deep learning scenarios.

1 Introduction

As the rise of deep learning, Stochastic Gradient Descent (SGD) has become one of the standard workhorses for optimizing deep models [5]. The study on the memorization of deep neural networks suggested the commonly used learning algorithms, e.g., SGD, played an important role of implicit regularization, where these algorithms prevent the over-parameterized models converging to the...
minimum points that cannot generalize well [31]. More specifically, for the SGD algorithm, it is believed that the inherent randomness, due to the random sampling strategies adopted, contributes to the implicit regularization effects of SGD [13, 33]. One direct evidence has been observed is that the large batch SGD typically performs worse than small batch ones [11, 16], since larger batch size reduces the randomness in SGD. Thus in order to further demystify of deep learning, understanding the randomness in SGD as well as its effect to generalization become critical.

Most of the previous research focused on studying the properties of SGD through modeling the algorithm as gradient descent (GD) with an unbiased noise term introduced by the random sampling. For example, [9, 15, 17] studied the mechanism of SGD noise on helping the learning dynamics escape from saddles and local minima. For neural networks with one hidden layer, the implicit regularization effect of SGD has been studied in [7]. Generalization bounds for stochastic gradient Langevin dynamics is obtained in [21], shedding light on the regularization role of SGD noise.

Yet another important line of understanding SGD is from the continuous-time perspective, where stochastic differential equations (SDEs) have been used as mathematical tools [23] to analyze SGD noise. The weak convergence between SGD and a continuous SDE is first established by [18], from which more efforts have been done to understand SGD and its noise [12, 13, 10]. To leverage the SGD noise, the work [11, 14] studied approaches to control the scale of SGD noise through tuning the batch sizes and learning rates. In addition to the noise scale, [33] studied the structure of the SGD noise, where the anisotropic property of SGD noise and its benefits on helping escape from (bad) local minima have been well examined. From the Bayesian perspective, the SDE based interpretation [19, 8, 27] further suggested that SGD indeed performs variational inference through entropy regularization which prevents over-fitting. Though SDE [18] offers a powerful tool for analyzing SGD mathematically, to what extent the approximation holds in practice is not fully understood. As a reference, the most recent study [26] argued that the SGD noise is heavy-tailed and non-Gaussian, thus it might not be the best tool to approximate SGD using SDE driven by Brownian motion.

Here we provide, for the first time, insights that understand the SGD noise from a mini-batch sampling perspective: instead of adopting the additive noise models, we proposed Multiplicative SGD (M-SGD) as a general case of SGD that models the stochastic gradient estimated per iteration of SGD using the matrix-vector product between a matrix of vertical gradient vectors, namely the gradient matrix, and a vector of random noises, namely the Multiplicative Noise (M-Noise). Compared with the traditional additive interpretation, M-Noise has the advantage of decoupling randomness from model parameters, shedding new lights on understanding SGD noise. Based on this novel perspective, we explicitly demonstrate the regularization effects of SGD, and introduce a fast algorithm to generate SGD-like noise to study the effects of SGD noise, and empirically verify the approximation between SGD and SDE [18]. Concisely, our main contributions are:

**Result I** - Our theoretical analysis on M-SGD shows that learning with SGD leads to an organic Structural Risk Minimization framework with a data-dependent regularizer resembling local Rademacher complexity. The finding thus explains the “implicit regularization” effects of SGD where the explicit regularization of SGD with local Rademacher complexity and the benefit of such regularization were studied in [30].

**Result II** - Beyond the weak convergence between SGD and SDE [18], which primarily relies on the moments information of SGD noise, we show that a special case of M-SGD with Gaussian M-Noise, namely M-SGD-Gaussian, holds strong convergence to the SDE.

**Result III** - Favorably, M-SGD model also provides us with an efficient way to approximate SGD with the noises of desired types, including the Gaussian noises based on either gradient covariance or Fisher matrices, where M-SGD is equipped with the M-Noise drawn from the interchangeable random distributions. Using this approach, we empirically verify that it is possible to approximate SGD noise by a Gaussian noise without loss of generalization performance, which supports our Result II.

**Result IV** - Moreover, we have empirically demonstrated that M-SGD could well approximate SGD with desired noises under practical mini-batch settings. We design a series of experiments systematically to show that, the M-Noise of SGD could be well approximated via 1) Bernoulli noise, 2) Gaussian noise with mini-batch estimated Fisher and 3) Sparse Gaussian noise. These results suggest the potential of using M-SGD to further develop practical learning algorithms.
2 M-SGD: Multiplicative Stochastic Gradient Descent

Machine learning problems usually involve minimizing an empirical loss over training data \{x_i, i = 1, \ldots, N\}, \(L(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(x_i; \theta)\), where \(\ell(x; \theta)\) is the loss over one example and \(\theta \in \mathbb{R}^D\) is the parameter to be optimized. Define the “loss vector” as \(L(\theta) := (\ell(x_1; \theta), \ldots, \ell(x_N; \theta)) \in \mathbb{R}^{1 \times N}\), then the gradient matrix is \(\nabla_\theta L(\theta) = (\nabla_\theta \ell(x_1; \theta), \ldots, \nabla_\theta \ell(x_N; \theta)) \in \mathbb{R}^{D \times N}\). Let \(\mathbb{1} := (1, \ldots, 1)^T \in \mathbb{R}^N\), then \(L(\theta) = \frac{1}{N} \sum_{i=1}^{N} \ell(x_i; \theta)\).

**SGD** The typical SGD iteration works as: it first randomly draws a mini-batch of samples with index set \(B_t = \{i_1, \ldots, i_b\}\), and then performs parameter update using the stochastic gradient \(\tilde{g}(\theta)\) estimated by the mini-batch and learning rate \(\eta\),

\[
\theta_{t+1} - \theta_t = -\eta \tilde{g}(\theta_t), \quad \tilde{g}(\theta_t) = \frac{1}{b} \sum_{i \in B_t} \nabla_\theta \ell(x_i; \theta_t).
\]

**Additive Noise (A-Noise)** Traditionally, the SGD noise is interpreted from additive viewpoint, i.e.,

\[
\tilde{g}(\theta_t) = \nabla_\theta L(\theta_t) + \mathcal{V}(\theta_t), \quad \mathcal{V}(\theta_t) := \tilde{g}(\theta_t) - \nabla_\theta L(\theta_t),
\]

where \(\mathcal{V}(\theta_t)\) represents the Additive-Noise (A-Noise) of SGD. We call the interpretation of SGD by Eq. (1) and Eq. (2) as Additive-Noise (A-SGD) model. Note that \(\mathcal{V}(\theta_t)\) might not be a Gaussian noise \([20]\), and its mean is zero and covariance is \(\text{Var}[\mathcal{V}(\theta_t)] = \frac{1}{b} \Sigma^{\text{a}}(\theta_t)\), where \(\Sigma^{\text{a}}(\theta) = \frac{1}{N} \nabla \ell(\theta) \nabla \ell(\theta)^T - \nabla L(\theta) \nabla L(\theta)^T\). Though commonly adopted in literature \([18, 33, 8, 19, 27, 14]\), it is clear the A-Noise \(\mathcal{V}(\theta)\) is dependent on the parameter \(\theta\), thus it varies along the optimization path, and causes trouble for understanding and analyzing. To overcome this obstacle, many works assumed that A-Noise is constant or upper bounded by some constant \([8, 14, 19, 32]\). Thus a natural question raises: could the noise in SGD be decoupled from parameters? Fortunately, our multiplicative noise provides a positive answer, as elaborated in the following.

**Multiplicative Noise (M-Noise)** By the definition of SGD, the randomness of SGD are indeed caused by the *mini-batch sampling* procedure, where this procedure is actually independent of current model parameter. Thus there should exist a parameter (i.e. \(\theta\))-independent model to characterize SGD noises rather than the aforementioned A-SGD. To this end, we propose the following formulation:

\[
\tilde{g}(\theta_t) = \nabla_\theta L(\theta_t) \cdot \mathcal{W}_{\text{sgd}},
\]

where \(\mathcal{W}_{\text{sgd}} \in \mathbb{R}^N\) is a random vector characterizing the *mini-batch sampling process*, i.e., for sampling without replacement, \(\mathcal{W}_{\text{sgd}}\) contains \(b\) multiples of \(\frac{1}{b} \mathbb{1}\) and \(N-b\) multiples of zero, with random index.

We hereby use *Multiplicative-Noise* (M-Noise) to denote \(\mathcal{W}_{\text{sgd}}\). Note that M-Noise is independent of parameter \(\theta\). The following Proposition 1 characterizes the properties of M-Noise of SGD.

**Proposition 1. (Mean and covariance of M-Noise in SGD)** For mini-batch sampled with replacement, the M-Noise \(\mathcal{W}_{\text{sgd}}\) in SGD satisfies

\[
\mathbb{E}[\mathcal{W}_{\text{sgd}}] = \frac{1}{N} \mathbb{1}, \quad \text{Var}[\mathcal{W}_{\text{sgd}}] = \frac{1}{bN} \left( I - \frac{1}{N} \mathbb{1} \mathbb{1}^T \right).
\]

For mini-batch sampled without replacement, the M-Noise \(\mathcal{W}'_{\text{sgd}}\) in SGD satisfies

\[
\mathbb{E}[\mathcal{W}'_{\text{sgd}}] = \frac{1}{N} \mathbb{1}, \quad \text{Var}[\mathcal{W}'_{\text{sgd}}] = \frac{N-b}{bN(N-1)} \left( I - \frac{1}{N} \mathbb{1} \mathbb{1}^T \right).
\]

Proof is left in Section 1.1 of the Appendix. We only consider the sampling with replacement case in the remaining parts, since most of our results hold for the other case, if not pointed out otherwise.

Besides SGD, we extend M-Noise to general cases and overload the notation M-SGD as:

\[
\theta_{t+1} - \theta_t = -\eta \nabla_\theta L(\theta_t) \cdot \mathcal{W}, \quad \mathbb{E}[\mathcal{W}] = \frac{1}{N} \mathbb{1}, \quad \mathcal{W} \in \mathbb{R}^{N \times 1}.
\]
Note that: 1) M-SGD becomes standard GD when \( \mathcal{W} = (\frac{1}{N}, \ldots, \frac{1}{N})^T \), and SGD if \( \mathcal{W} = \mathcal{W}_{\text{sgd}} \).

2) The M-Noise \( \mathcal{W} \) is independent of model, parameter and dataset. Such decoupling provides us with a clear picture at the regularization effect of SGD. We will elaborate this point in next section. 3) One special case we would like to pay more attention is when \( \mathcal{W} \) is a Gaussian noise, i.e., \( \mathcal{W}_\text{G} \sim \mathcal{N}(\frac{1}{N}, \Sigma) \), and we call Eq. (6) M-SGD-Gaussian. Our analysis will later show that there is a strong approximation of the discrete M-SGD-Gaussian by continuous SDE [18]. Moreover, we will empirically demonstrate that approximating \( \mathcal{W}_{\text{sgd}} \) by \( \mathcal{W}_\text{G} \) achieves highly similar regularization effects. Thus it is meaningful to use SDE as a tool for understanding the generalization benefits of SGD and its variants.

### Connection between A-Noise and M-Noise

Let M-Noise \( \mathcal{W} = \frac{1}{N} \mathbb{I} + \mathcal{V} \), then we have the corresponding A-Noise \( \mathcal{V}(\theta) = \nabla_\theta \mathcal{L}(\theta) \mathcal{V} \). Moreover, under the assumption that \( \mathcal{V}(\theta) \) follows a Gaussian distribution, then \( \mathcal{W} \) is Gaussian too. This property plays a crucial role for us to design fast algorithm injecting noise into gradient based algorithms as shown in Section 5.1. Though A-Noise and M-Noise could convert between each other, M-Noise decouples noise and parameter, which gives us new insights on the behavior of SGD. For example, we now make use of M-Noise perspective to explicitly elaborate the implicit bias of SGD.

### 3 M-SGD Performs Data-Dependent Regularization

This section presents details of Result I. Let us first recall \( L(\theta) = \frac{1}{N} \mathcal{L}(\theta) \mathbb{I} \). In Eq. (9), let \( \mathcal{W} = \frac{1}{N} \mathbb{I} + \frac{1}{N} \mathcal{V} \), \( \mathcal{V} = (v_1, \ldots, v_N)^T \) and rewrite it as

\[
\theta_{k+1} - \theta_k = -\eta \nabla_\theta L(\theta_k) - \eta \nabla_\theta \left( \frac{1}{N} \mathcal{L}(\theta_k) \cdot \mathcal{V} \right) = -\eta \nabla_\theta \left( \mathcal{L}(\theta_k) + \frac{1}{N} \mathcal{L}(\theta_k) \mathcal{V} \right), \quad \mathbb{E}[\mathcal{V}] = 0. \quad (7)
\]

Thus learning \( L(\theta) \) by M-SGD equals to applying GD to optimize the objective \( L(\theta) \) with a randomized data-dependent regularization term:

\[
\tilde{L}(\theta) := L(\theta) + \frac{1}{N} \mathcal{L}(\theta) \mathcal{V} = \frac{1}{N} \sum_{i=1}^N \ell(x_i; \theta) + \frac{1}{N} \sum_{i=1}^N v_i \ell(x_i; \theta)
\]

\[
\leq \frac{1}{N} \sum_{i=1}^N \ell(x_i; \theta) + \frac{1}{N} \sup_{\|\theta' - \theta\|_2 \leq \delta} \left| \sum_{i=1}^N v_i \ell(x_i; \theta') \right|
\]

(8)

We upper bound the random term in M-SGD by its local maximum in \( \delta \)-ball, and as \( \delta \to 0 \) the inequality becomes tighter. The right hand side of the objective function (8) could be treated as the empirical realization of the population objective (9):

\[
\tilde{L}_{\text{popu}}(\theta) := \mathbb{E}_x[\ell(x; \theta)] + \mathbb{E}_{x_1, \ldots, x_N} \mathbb{E}_\mathcal{V} \left[ \frac{1}{N} \sup_{\|\theta' - \theta\|_2 \leq \delta} \left| \sum_{i=1}^N v_i \ell(x_i; \theta') \right| \right].
\]

(9)

The explicit regularization of SGD with the local Rademacher complexity with a \( \delta \)-ball, and the empirical benefit of such regularization in image classification and neural network architecture search have been reported in [30]. The difference is that we show that SGD has an implicit regularization resembling local Rademacher complexity.

We denote \( R(\mathcal{V}, \theta, \delta, N) := \mathbb{E}_{x_1, \ldots, x_N} \mathbb{E}_\mathcal{V} \left[ \frac{1}{N} \sup_{\|\theta' - \theta\|_2 \leq \delta} \left| \sum_{i=1}^N v_i \ell(x_i; \theta') \right| \right] \). For any M-Noise \( \mathcal{V}, R(\mathcal{V}, \theta, \delta, N) \) defines a local complexity measure.

Note that the components of \( \mathcal{V} \) might not be independent. Specially, 1) for \( \mathcal{A} = (a_1, \ldots, a_N)^T \) and \( a_i, i = 1, \ldots, N \) be i.i.d., \( \mathbb{P}[a_i = 1] = \mathbb{P}[a_i = -1] = \frac{1}{2} \), \( R(\mathcal{A}, \theta, \delta, N) \) is the local Rademacher complexity [2, 1, 3, 30]; 2) let \( \mathcal{G} = (g_1, \ldots, g_N)^T \sim \mathcal{N}(0, I) \), then \( R(\mathcal{G}, \theta, \delta, N) \) is the local Gaussian complexity [12], which is the corresponding regularization term of M-SGD-Gaussian with independent Gaussian M-Noise; 3) for SGD noise \( \mathcal{V}_{\text{sgd}} \), we name \( R(\mathcal{V}_{\text{sgd}}, \theta, \delta, N) \) the local SGD complexity.

We provide the following results to bound local Rademacher, Gaussian and SGD complexity.

\[\text{[In literature, some define Rademacher/Gaussian complexity with absolute sign and some without. This does not cause big difference for obtaining generalization bound, and we adopt the one with absolute sign.]}

Theorem 1. (Local Rademacher, Gaussian and SGD complexity) Let \( A, G, V_{s gd} \) be the Rademacher, Gaussian and SGD random variables, respectively. Then there exist \( c, C > 0 \) such that:

\[
\begin{align*}
(1) \quad & cR(A, \theta, \delta, N) \leq R(G, \theta, \delta, N) \leq C \ln N \cdot R(A, \theta, \delta, N), \\
(2) \quad & R(V_{s gd}, \theta, \delta, N) \leq \frac{2(k-1)}{k} R(A, \theta, \delta, b), \quad \text{if } N = kb, k \in \mathbb{N}, k > 1.
\end{align*}
\]

The proof can be found in Sections 1.2 and 1.3 of the Appendix.

Theorem 1 tells us that local Gaussian complexity is equivalent to local Rademacher complexity, which explains the generalization advantage of M-SGD-Gaussian, since regularizing Rademacher complexity is known to bring benefits for generalization [22, 20, 8]. Though we cannot build perfect bridge between local SGD complexity and local Rademacher complexity yet, in Section 5 we will show that M-SGD-Gaussian could perfectly simulate SGD, given proper covariance of the Gaussian M-Noise. Thus we conclude that the local SGD complexity works similar to local Gaussian complexity and local Rademacher complexity, and the implicit bias of SGD is due to this data-dependent complexity regularizer.

Figure 1 (a)(d) show empirical comparison of the generalization performance of GD, SGD, M-SGD, and GD optimizing loss with Rademacher regularizer. We can clearly observe that SGD and M-SGD family function similarly to GD-Rademacher, thus supporting our understanding on the data-dependent regularization effect of SGD and M-SGD.

4 The Continuous Approximation of M-SGD

This section primarily focus on presenting Result II of our work. With the implicit bias of M-SGD known, we now address the issue of its continuous approximation. We first recollect the weak approximation between discrete A-SGD and continuous SDE [13, 12, 10].
Heuristically, let $dt \approx \eta$ and $dW_t \approx \sqrt{\eta \epsilon} \epsilon \sim \mathcal{N}(0, I)$, A-SGD iteration \( [1][2] \) could be treated as a discretization of the following SDE

$$d\theta_t = -\nabla g(\theta_t) dt + \sqrt{\frac{\eta}{b} \Sigma_{\text{sgd}}(\theta_t)} dW_t.$$  \( \tag{12} \)

It is important to recognize the noises driving A-SGD iteration \( [1][2] \) and SDE \( [12] \) are independent processes, hence we could only understand the approximation between them in a weak sense.

**Theorem 2.** (Weak convergence between A-SGD and SDE \( [18] \)) Let $T \geq 0$. Under mild assumptions, SGD \( [1] \) is an order 1 weak approximation of the SDE \( [12] \), i.e., for a general class of test function $g$,

$$\|E_g(\theta_{k\eta}) - E_g(\theta_k)\| \leq C \eta$$ for all $0 \leq k \leq \lfloor T/\eta \rfloor$. \( \tag{13} \)

Please refer to Theorem 1 in \( [18] \) for the rigorous statement and proof.

Similarly, the weak approximation also holds for M-SGD \( [1][3] \), given the corresponding M-Noise shares the same covariance with the multiplicative noise of SGD, since Theorem 2 only makes use of the moments of SGD noise. The weak convergence provides us with the equivalence of the discrete iteration and the continuous SDE in sense of probability distributions. Nonetheless, the path-wise closeness between the two processes is not ensured.

**M-SGD-Gaussian.** To obtain stronger approximation, e.g., path-wise convergence, we need to make assumption that M-Noises are drawn from a Gaussian distribution, i.e., M-SGD-Gaussian. Concisely, Theorem 3 guarantees the strong convergence between M-SGD-Gaussian and SDE \( [12] \).

**Theorem 3.** (Strong convergence between M-SGD-Gaussian and SDE) - Let $T \geq 0$. Assume $\ell_i(\theta)$ are bounded with uniformly Lipschitz continuous gradients for all $i = 1, 2, ..., N$. Then Eq. \( [12] \) is an order 1 strong approximation of M-SGD-Gaussian Eq. \( [6] \), i.e.,

$$E\|\theta_{k\eta} - \theta_k\|^2 \leq C \eta^2$$ for all $0 \leq k \leq \lfloor T/\eta \rfloor$. \( \tag{14} \)

The rigorous statement and proof are deferred to Section 1.4 in the Appendix.

The strong convergence guarantees the path-wise closeness between $\theta_k$ and $\theta_{k\eta}$, which indicates the close behavior not only at the level of probability distributions but also at the level of sample paths of the two processes. In Section 5 (Figure 1(a)(d)), we will empirically verify that M-SGD-Gaussian achieves highly similar regularization effects as SGD, which makes it reasonable to understand SGD via M-SGD-Gaussian and its strong approximation, the continuous SDE.

## 5 The Discrete Approximation of SGD using M-SGD

In this section we study the way to approximate SGD using M-SGD with M-Noise drawn from interchangeable random distributions with/without mini-batch settings. Compared to A-SGD, our proposed M-SGD can easily generate noises of various useful and desired types with low computational complexity, using the M-Noise drawn from interested distributions. In the rest of this section, we first introduce the fast algorithm for implementing M-SGD-Gaussian, then present the details about Result III and Result IV, all based on the Fast M-SGD-Gaussian Algorithm and its variants.

### 5.1 Fast M-SGD-Gaussian: efficient Gaussian noise generation with gradient covariance

Approximating the noise in SGD by a Gaussian one is a common used trick \( [33][14][29] \). The targeted noise is a Gaussian noise with gradient covariance $\frac{1}{b} \Sigma_{\text{sgd}}(\theta)$, denoted as $\nu$. To obtain such noise, one would first compute the covariance matrix and then apply the singular value decomposition (SVD), $\Sigma_{\text{sgd}}(\theta) = U(\theta)\Lambda(\theta)U(\theta)^T$, to transform a white noise $\epsilon$ into the noise desired, $\nu = \frac{1}{\sqrt{b}} U(\theta) \Lambda(\theta) \tilde{\epsilon}$.

However there are two obstacles in the above generation procedures: 1) evaluating and storing $\Sigma_{\text{sgd}}(\theta) \in \mathbb{R}^{D \times D}$ is computationally unacceptable, with both $N$ and $D$ being large; 2) performing SVD for a $D \times D$ matrix is comprehensively hard when $D$ is extremely large. Furthermore, one needs to repeat 1) and 2) at every parameter update step, since $\Sigma_{\text{sgd}}(\theta)$ depends on parameter $\theta$. In compromise, current works suggest to approximate gradient covariance using only its diagonal or block diagonal elements \( [29][33][14][20] \). Generally, there is no guarantee that the diagonal information could approximate full gradient covariance well. Specifically, \( [33] \) empirically showed that such diagonal approximation cannot fully recover the regularization effects of SGD. Thus a more effective approach of generating Gaussian noise with gradient covariance is of both theoretical and empirical importance.
Inspired by M-SGD framework (6), we propose a fast algorithm to generate Gaussian-like SGD noise. First of all, through a little calculation it can be shown that

$$
\Sigma_{\text{sgd}}(\theta) = \frac{1}{N} \left( \nabla_{\theta} \mathcal{L}(\theta) \left( I - \frac{1}{N} I \right)^T \right) \left( \nabla_{\theta} \mathcal{L}(\theta) \left( I - \frac{1}{N} I \right)^T \right)^T. 
$$

(15)

In this way, the preferred Gaussian noise could be sampled as $\nu = \frac{1}{\sqrt{bN}} \nabla_{\theta} \mathcal{L}(\theta) \left( I - \frac{1}{N} I \right)^T \epsilon$.

Besides, since $\nabla_{\theta} L(\theta) = \frac{1}{N} \nabla_{\theta} \mathcal{L}(\theta) I$, we indeed can borrow M-SGD-Gaussian as the approximation of SGD with Gaussian noises such that

$$
\theta_{t+1} - \theta_t = -\eta \nabla_{\theta} L(\theta_t) - \eta \nu = -\eta \nabla_{\theta} \mathcal{L}(\theta_t) I - \eta \frac{1}{\sqrt{bN}} \nabla_{\theta} \mathcal{L}(\theta_t) \left( I - \frac{1}{N} I \right)^T \epsilon
$$

$$
= -\eta \nabla_{\theta} \mathcal{L}(\theta_t) \cdot \mathcal{W}_G, \quad \mathcal{W}_G = \frac{1}{N} + \frac{1}{\sqrt{bN}} \left( I - \frac{1}{N} I \right)^T \epsilon, \quad \epsilon \sim \mathcal{N}(0, I). 
$$

(16)

**Fast Implementation** Thanks to the linearity of derivation operator and the feasibility of derivation operator to communicate with weight average operator, we can design the fast algorithm (described in Algorithm [16] to implement M-SGD-Gaussian (in the form of Eq. (16)).

**Algorithm 1** Fast Implementation of M-SGD-Gaussian (16)

1: **Input:** Input initialization $\theta_0 \in \mathbb{R}^D$, training samples $(x_1, y_1), \ldots, (x_N, y_N)$, loss function

   $\ell_i(\theta) = \ell((x_i, y_i), \theta)$, loss vector $\mathcal{L}(\theta) = (\ell_1(\theta), \ldots, \ell_N(\theta))$, random noise $\epsilon \sim \mathcal{N}(0, I_{N \times N})$, learning rate $\eta > 0$

2: for $k = 0, 1, 2, \ldots, K - 1$

3: Generate random weight $\mathcal{W}_G = \frac{1}{N} I + \frac{1}{\sqrt{bN}} \left( I - \frac{1}{N} I \right)^T \epsilon, \epsilon \sim \mathcal{N}(0, I_{N \times N})$

4: Calculate randomized loss $\tilde{L}(\theta_k) = \mathcal{L}(\theta_k) \cdot \mathcal{W}_G \in \mathbb{R}$

5: Compute noisy gradient $\nabla_{\theta} \tilde{L}(\theta_k) = \nabla_{\theta} (\mathcal{L}(\theta_k) \cdot \mathcal{W}_G)$

6: Update parameter $\theta_{k+1} = \theta_k - \eta \nabla_{\theta} \tilde{L}(\theta_k)$

7: end for

8: **Output:** Output $\theta_K$

**Remark:** 1) Before the deep learning era, the typical setting of machine learning is $N \gg D$, i.e., the number of samples is larger than that of parameters. In this circumstance, the SVD way of generating Gaussian noise is indeed plausible. However, when it comes to deep networks where $N \ll D$, or both numbers are high, it turns out computing the full gradient could be far less efficient than explicitly evaluating the covariance matrix and performing SVD, resulting in the computational advantage of our method over the traditional one. 2) Our method could be easily extended to generate other types of noise besides Gaussian, e.g., Bernoulli noise and the mini-batch version of noises. See the following for more discussions.

5.2 **Approximate the M-Noise of SGD by Gaussian ones and components independent ones**

Here, we present the details of Result III. First, based on the Fast M-SGD-Gaussian (16), we unify two types of commonly used Gaussian noise for simulating SGD’s behavior: Gaussian noise with gradient covariance (M-SGD-Cov) (33) and Gaussian noise with Fisher (M-SGD-Fisher) (29).

**M-SGD-Cov and M-SGD-Fisher** First we know $\Sigma_{\text{sgd}}(\theta) = F(\theta) - \nabla_{\theta} L(\theta) \nabla_{\theta} L(\theta)^T$, where

$$
F(\theta) = \frac{1}{N} \nabla_{\theta} \mathcal{L}(\theta) \nabla_{\theta} \mathcal{L}(\theta)^T
$$

is the Fisher. Intuitively, M-SGD-Cov and M-SGD-Fisher should not be far away from each other. We can see this using SDE (12). At the beginning stage of SGD training, the drift term outlarges the diffusion term in scale (33) (25), dominates the optimization, and the noise term almost makes no contribution, no matter whether it is gradient covariance noise or Fisher noise. During the latter diffusion stage, however, the gradient terms to be close to zero, thus $\Sigma_{\text{sgd}}(\theta) \approx F(\theta)$. In a nutshell, covariance noise and Fisher noise should behave similarly for regularizing SGD iteration.

Thanks to M-SGD-Gaussian formulation, we could now give a mathematical analysis on the difference between these two types of noise. Let $\mathcal{W}_F$ and $\mathcal{W}_{\text{Cov}}$ be the M-Noises for generating Fisher noise and
gradient covariance noise, respectively, then from Eq. (15) and Eq. (16), we have:

\[ \mathcal{W}_{\text{Cov}} = \frac{1}{N} + \frac{1}{\sqrt{bN}} \left( I - \frac{1}{N} 11^T \right) \epsilon, \quad \mathcal{W}_F = \frac{1}{N} + \frac{1}{\sqrt{bN}} \epsilon, \quad \epsilon \sim \mathcal{N}(0, I). \]  

(17)

Note that matrix \( \left( I - \frac{1}{N} 11^T \right) \) centralizes a random vector. Thus the M-SGD perspective tells us the only difference between \( \mathcal{W}_{\text{Cov}} \) and \( \mathcal{W}_F \) is that, in the former one, the white noise for generating the M-Noise is firstly processed by centralization. On the other hand, since the components of \( \epsilon \in \mathbb{R}^N \) are already identically distributed with zero mean, and \( N \) is extremely large in deep learning with huge training data, thus \( \frac{1}{\sqrt{bN}} \epsilon \approx 0 \) and the centralization procedure barely does anything to the white noise, i.e., \( \epsilon \approx \left( I - \frac{1}{N} 11^T \right) \epsilon \). Therefore \( \mathcal{W}_{\text{Cov}} \approx \mathcal{W}_F \) along the whole optimization path, which leads to identical regularization effect for learning deep models.

**M-SGD-Bernoulli** To further verify our observation, we introduce M-SGD-Bernoulli that employs Bernoulli M-Noise to approximate the behaviors of the SGD with its diagonal (part of) M-Noise covariance matrix, i.e., \( \text{diagVar}[\mathcal{W}_{\text{sgd}}] \). Consider a random vector \( \mathcal{W}_b = (w_1, \ldots, w_N)^T \), \( \mathbb{P}(w_i = \frac{1}{N} + \frac{1}{\sqrt{b}}) = \frac{1}{N}, \mathbb{P}(w_i = \frac{1}{N}) = \frac{N b}{N b}, \) \( w_i \) i.i.d. Then \( \mathbb{E}[\mathcal{W}_b] = \frac{1}{N} \mathbb{I} \) and \( \text{Var}[\mathcal{W}_b] = \frac{N b - 1}{N b^2} \mathbb{I} = \text{diagVar}[\mathcal{W}_{\text{sgd}}] \). In this way, we can see that the covariance of Bernoulli M-Noise is the diagonal of the covariance of SGD M-Noise. Note that this “diagonal” relationship might not hold for their corresponding A-Noises. This Bernoulli M-Noise could be viewed as the best approximation of SGD M-Noise, among all the random variables with independent components.

**Results and Observations** The experiment results shown in Figures 1(a)(d) demonstrate that, under the same settings, M-SGD-Fisher and M-SGD-Cov algorithms perform almost the same, while the performance of M-SGD-Bernoulli tightly follows up the previous two. Together with our theoretical insights from M-SGD perspectives, we can conclude that 1) gradient covariance should be equivalent to the Fisher for SGD (validating our theoretical findings), and 2) the M-Noise of SGD \( \mathcal{W}_{\text{sgd}} \) could be well approximated by noises with independent components, e.g., \( \mathcal{W}_b \) and \( \mathcal{W}_F \).

### 5.3 Practical SGD approximation using mini-batch M-SGD

**M-SGD-[Fisher-b] and M-SGD-[Cov-b]** To derive our results step by step, we first introduce two intermediate results based on M-SGD-[Fisher-b] or M-SGD-[Cov-b]. Such M-SGD variants approximate the behaviors of SGD that use mini-batch estimated gradient covariance or Fisher matrices to generate Gaussian random noises and the bath size is \( b \). The implementation of these two algorithms are addressed in Section 2 of the Appendix. Note that, though using mini-batch gradients to estimate Fisher/covariance matrix, the generated M-Noises [17] are not sparse since it is still the summation of a constant and a Gaussian noise.

**[M-SGD-Fisher]-b and [M-SGD-Cov]-b** We further define the mini-batch versions of M-SGD-Fisher and M-SGD-Cov. The M-Noises defined to be the composition of a mini-batch sampling random variable (with batch size \( b \)) and a Gaussian random variable. Thus the M-Noises are sparse Gaussian with \( b \) non-zero Gaussian random elements. In this way, \( b \) naturally becomes the batch size of M-SGD, as the gradients corresponding to the zero elements in the M-Noise vector would be ignored in matrix-vector product. Please refer to Section 2 of Appendix for implementation details. Note that these algorithms lower the computational complexity of M-SGD using only mini-batch of data for the parameter update per iteration.

**Results and Observations** Under the settings of \( b \ll N \ll D \), estimating a \( D \times D \) gradient covariance/Fisher matrix with a batch of gradients should be difficult. To our surprise again the experimental results shown in Figures 1(b)(e) demonstrate that the generalization performances of M-SGD-[Fisher-b] and M-SGD-[Cov-b] are close to M-SGD-Fisher and M-SGD-Cov, which estimate the gradient covariance and Fisher matrices using full gradients. Furthermore, Figures 1(c)(f) exhibit that testing accuracy of [M-SGD-Fisher]-b and [M-SGD-Cov]-b could still be maintained, even when the M-Noises are sparse, indicating the strong application prospects of M-SGD.

**Large Batch Training** Especially, when the batch size becomes large, the generalization of vanilla SGD would be hurt and perform even worse than the SGD with small batch size [11][16]. In the same Figures 1(c)(f), our experiments show that M-SGD with various M-Noise settings can still recover the generalization performance under the same large batch settings (\( b=2000 \) or \( 5000 \) with ghost batch normalization, learning rate tuning, and regime adaptation) [11]. Thus, our perspective of multiplicative SGD might shed new light on developing new algorithm of large batch training.
maintaining both the speed advantage and generalization guarantee. We leave further investigation along this direction as future work.

6 Discussions and Conclusions

In this work, we introduce Multiplicative SGD model (M-SGD) to interpret the randomness of SGD, from Multiplicative Noise (M-Noise) perspectives. First of all, we find the M-Noise helps establish a theory that connects the generalization of SGD to a data-dependent regularizer of Rademacher complexity type. Moreover, under the known Gaussian M-Noise assumptions, the M-SGD model holds a strong convergence to the known SDE of SGD, beyond the weak convergence obtained in [13]. In addition, based on M-SGD formulation a fast algorithm is developed to efficiently insert noise into gradient descent. Using the algorithm, we empirically verify that M-SGD with various desired types of M-Noises can well approximate the behaviors of SGD, in the sense of achieving similar generalization performance. Compared to the traditional analytical models based on the additive noise, we find multiplicative noises provides an alternative way to understand SGD, with insightful new results for both theory and application.

As the first work along the M-Noise road, there are several unsolved theoretical challenges, e.g., the relationship between local Rademacher complexity and local SGD complexity, and more general local complexity measures. These open problems are left for future work.

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The contributions of the authors are the following: JW came up with the core ideas, contributed to the proof of Theorem 1, implemented all the experiments and wrote most part of the paper. WH contributed to the proof of Theorems 1, 2 and participated in paper writing. HX led the research discussions with JW as an intern in Baidu Research and wrote part of this paper. JH participated in the discussion and wrote part of the paper. ZZ led the research on studying the behavior of SGD. With JW he jointly proposed and discussed research agenda on the multiplicative noise of SGD, proposed the core idea of Section 3, and wrote part of the paper.

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A Missing Proofs in Main Paper

A.1 Proof of Proposition 1

Proof. Sampling without replacement

By definition, the random variable $W_{sgd}$ could be decompose as

$$W_{sgd} = W^1 + \cdots + W^b,$$

where $W^i, i = 1, \ldots, b$ are i.i.d, and they represent once sampling procedure. Thus $W^i = (w^i_1, \ldots, w^i_N)^T$ contains one $\frac{1}{b}$ and $N-1$ zeros, with random index. By its definition, we know

$$E[w^i_j] = \frac{1}{bN}, \quad \forall j$$

$$E[w^i_j w^i_j] = \frac{1}{b^2N}, \quad \forall j$$

$$E[w^i_j w^i_k] = 0, \quad \forall j \neq k.$$

Thus

$$E[W^i] = \frac{1}{bN} 1$$

$$\text{Var}[W^i] = E[W^i (W^i)^T] - E[W^i]E[W^i]^T$$

$$= \begin{pmatrix} \frac{1}{b^2N} & \cdots & \frac{1}{b^2N} \\ \vdots & \ddots & \vdots \\ \frac{1}{b^2N} & \cdots & \frac{1}{b^2N} \end{pmatrix} - \frac{1}{b^2N^2} 1 1^T$$

$$= \frac{1}{b^2N} \left( I - \frac{1}{N} 1 1^T \right).$$

Because $W^i, i = 1, \ldots, b$ are i.i.d., we have

$$E[W] = bE[W^i] = \frac{1}{N} 1$$

$$\text{Var}[W] = b\text{Var}[W^i] = \frac{1}{bN} \left( I - \frac{1}{N} 1 1^T \right).$$

Sampling with replacement
Let $W'_{\text{sgd}} = (w'_1, \ldots, w'_N)^T$, by definition, $W'_{\text{sgd}}$ contain $b\frac{1}{b}$s and $N - b$ zeros, with random index. Thus

$$E[w'_j] = \frac{(N-1)b}{b(N)} = \frac{1}{N}, \quad \forall j$$

(28)

$$E[(w'_j)^2] = \frac{(N-1)b}{b(N)} = \frac{1}{bN}, \quad \forall j$$

(29)

$$E[w'_j w'_k] = \frac{(N-2)b}{b(N)} = \frac{b - 1}{bN(N - 1)}, \quad \forall j \neq k.$$  

(30)

Hence

$$E[W'_{\text{sgd}}] = \frac{1}{N}I$$

(31)

$$\text{Var}[W'_{\text{sgd}}] = E[W'_{\text{sgd}}(W'_{\text{sgd}})^T] - E[W']E[W']^T$$

(32)

$$= \begin{pmatrix}
\frac{1}{bN(N-1)} & \frac{1}{bN} & \cdots & \frac{1}{bN(N-1)} \\
\frac{1}{bN} & \frac{1}{bN} & \cdots & \frac{1}{bN} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{1}{bN(N-1)} & \frac{1}{bN} & \cdots & \frac{1}{bN}
\end{pmatrix} - \frac{1}{N^2}I^T$$

(33)

$$= \frac{N - b}{bN(N - 1)} \left( I - \frac{1}{N} \frac{1}{N}^T \right)$$

(34)

$$= \frac{N - b}{bN(N - 1)} \left( - \frac{1}{N} \frac{1}{N}^T \right)$$

(35)

A.2 Proof of Theorem 1: first half

Define the Rademacher variables $a_1, \ldots, a_N \in \{1, -1\}$ with even probability. Define the standard Rademacher complexity

$$R(A, \theta, \delta, N) = \frac{1}{N}E_{x_1, \ldots, x_N}E_{a_1, \ldots, a_N} \sup_f \left| \sum_{i=1}^{N} a_i f(x_i) \right|.$$  

(36)

Let $g_1, \ldots, g_N$ be a sequence of independent $\mathcal{N}(0, 1)$ Gaussian random variables. Define the Gaussian Rademacher complexity

$$R(G, \theta, \delta, N) = \frac{1}{N}E_{x_1, \ldots, x_N}E_{g_1, \ldots, g_N} \sup_f \left| \sum_{i=1}^{N} g_i f(x_i) \right|.$$  

(37)

Theorem (The first part of Theorem 1 in the paper, Lemma 4 in [2]). There are absolute positive constants $c$ and $C$ such that

$$cR(A, \theta, \delta, N) \overset{(38)}{\leq} R(G, \theta, \delta, N) \overset{(38)}{\leq} C \ln N \cdot R(A, \theta, \delta, N).$$

(38)

Proof. The proof follows [28, 24]. Indeed, our proof holds for not only local Rademacher and Gaussian complexity, but also original Rademacher and Gaussian complexity. Thus for the simplicity of notations, we omit $\theta$ in function $f$ and write $\sup_{\|\theta - \theta'\| \leq \delta} f(x; \theta')$ as $\sup_{f} f(x)$.
We first prove the inequality (38a). Set $\mu$ be the product probability measure on $\mathbb{R}^N$ and let $b \equiv \mathbb{E}|g_i| = \int |g_i| \, d\mu$, note that $g_i$ and $-g_i$ are identical distributed. Then

$$\mathbb{E}_{a, \sup_f} \sum a_i f(x_i) \tag{39}$$

and let $b \equiv \mathbb{E}|g_i| = \int |g_i| \, d\mu$, note that $g_i$ and $-g_i$ are identical distributed. Then

$$\mathbb{E}_{a, \sup_f} \sum a_i f(x_i) \tag{39}$$

Let us now demonstrate (38b). To this end we first propose the following estimate [24]. If $0 \leq \alpha_i \leq 1$, then

$$\mathbb{E}_{a, \sup_f} \sum_{i=1}^N \alpha_i f(x_i) \leq \mathbb{E}_{a, \sup_f} \sum_{i=1}^N a_i f(x_i) \tag{48}$$

If we apply (48) to $\alpha_i = \frac{|g_i|}{\max_{i=1,\ldots,N} |g_i|}$, then we get

$$\mathbb{E}_{a, \sup_f} \sum_{i=1}^N a_i |g_i| f(x_i) \leq \left( \max_{i=1,\ldots,N} |g_i| \right) \cdot \mathbb{E}_{a, \sup_f} \sum_{i=1}^N a_i f(x_i) \tag{49}$$

and thus

$$\mathbb{E}_{g_i, \sup_f} \sum_{i=1}^N g_i f(x_i) = \mathbb{E}_{g_i, \sup_f} \sum_{i=1}^N a_i g_i f(x_i) \tag{50}$$

(since $g_i$ and $-g_i$ are identically distributed)

$$\leq \left( \mathbb{E}_{g_i, \sup_f} \max_{i=1,\ldots,N} |g_i| \right) \cdot \mathbb{E}_{a, \sup_f} \sum_{i=1}^N a_i f(x_i) \tag{51}$$

so that we conclude (38b) by noticing that $\mathbb{E}_{g_i, \sup_f} \max_{i=1,\ldots,N} |g_i| \leq C \ln N \tag{52}$ (55, Lemma 11.3).
It remains to show (48). Due to the absolute sign inside the sup and the symmetry, without loss of generality we can always assume that $a_1 = 1$. If $N = 2$, we are left to show that
\[
\frac{1}{2} \sup_f |\alpha_1 f(x_1) + \alpha_2 f(x_2)| + \frac{1}{2} \sup_f |\alpha_1 f(x_1) - \alpha_2 f(x_2)| \leq \frac{1}{2} \sup_f |f(x_1) + f(x_2)| + \frac{1}{2} \sup_f |f(x_1) - f(x_2)|.
\]

(53)

We can fix $\alpha_1$ and consider the function $F(\alpha_1, \alpha_2) = \frac{1}{2} \sup_f |\alpha_1 f(x_1) + \alpha_2 f(x_2)| + \frac{1}{2} \sup_f |\alpha_1 f(x_1) - \alpha_2 f(x_2)|$. It can be directly verified that $F(\alpha_1, \alpha_2)$ is convex in $\alpha_2$, since it is the summation of two convex function in $\alpha_2$. Also $F(\alpha_1, \alpha_2) = F(\alpha_1, -\alpha_2)$, and thus for any $0 \leq \alpha_2 \leq 1$ we have $F(\alpha_1, \alpha_2) \leq F(\alpha_1, 1)$. In a same way $F(\alpha_1, 1) \leq F(1, 1)$, and we conclude (48) for $N = 2$.

The case for general $N$ follows the same idea by introducing the function
\[
F(\alpha_1, \ldots, \alpha_N) = \frac{1}{2^{N-1}} \sum \sup_{\text{all } 2^{N-1} \text{ combinations of } (1, \pm 1, \ldots, \pm 1)} |\alpha_1 f(x_1) \pm \alpha_2 f(x_2) \pm \ldots \pm \alpha_N f(x_N)|,
\]

and iteratively $F(\alpha_1, \ldots, \alpha_N) \leq F(1, \alpha_2, \ldots, \alpha_N) \leq F(1, 1, \ldots, \alpha_N) \leq \ldots \leq F(1, 1, \ldots, 1)$, which is (48).

In summary we finish the proof. \qed

A.3 Proof of Theorem 1 second half

Let $V = (v_1, \ldots, v_N)^T$ be the M-Noise of SGD, by definition we know that for $V$, the number of $\frac{N}{k} - 1$ is $b$ and the number of $-1$ is $N - b$. For simplicity, let $N = kb, k \in \mathbb{N}, k > 1$. Thus in $V$, the number of $k - 1$ is $b$ and the number of $-1$ is $(k - 1)b$.

**Theorem** (The second part of Theorem 1 in the paper). Assume $N = kb, k \in \mathbb{N}, k > 1$, then
\[
R(V, \theta, \delta, bk) \leq \frac{2(k-1)}{k} R(A, \theta, \delta, b).
\]

(55)

**Proof.** First we know that for i.i.d. examples $x_i, i = 1, \ldots, N$, the following equation holds for any function $F$:
\[
\mathbb{E}_{x_1,\ldots,x_N} F(x_1, \ldots, x_N) = \mathbb{E}_{x_1,\ldots,x_N} F(x_{i_1}, \ldots, x_{i_N}),
\]

(56)

where $i_1, \ldots, i_N$ is a permutation of $1, \ldots, N$.

Thus by definition of SGD complexity
\[
R(V, \theta, \delta, N) = \frac{1}{N} \mathbb{E}_x \mathbb{E}_{v_1} \sup_f \left| \sum_{i=1}^{N} v_i f(x_i) \right|
\]

(57)

and the definition of M-Noise $V = (v_1, \ldots, v_N)^T$, i.e., the number of $\frac{N}{k} - 1$ is $b$ and the number of $-1$ is $N - b$ at any cases, we could permute the index of $x_i$, such that $v_1, \ldots, v_b = \frac{N}{k} - 1, v_{b+1}, \ldots, v_N = -1$, without affecting the SGD complexity. Thus we have
\[
R(V, \theta, \delta, N) = \frac{1}{N} \mathbb{E}_x \sup_f \left| \left( \frac{N}{b} - 1 \right) (f(x_1) + \cdots + f(x_b)) - (f(x_{b+1}) + \cdots + f(x_N)) \right|
\]

(58)
Then the M-SGD-Gaussian iteration (67)

Theorem. (Rigorous statement of Theorem 3: Strong convergence between M-SGD-Gaussian and SDE) Let $\Theta$ be the diffusion matrix, e.g., $C(\Theta) = \frac{\sqrt{DB}C(\Theta)}{\sqrt{N}} \in \mathbb{R}^{D \times N}$. Assume there exist some $L, M > 0$ such that $\max_{i=1,2,...,N} \max_{x} (|\nabla \ell_i(x)|) \leq M$ and that $\nabla \ell_i(x)$ are Lipschitz continuous with bounded Lipschitz constant $L > 0$ uniformly for all $i = 1, 2, ..., N$.

Then the M-SGD-Gaussian iteration (67)

$$\theta_{k+1} - \theta_k = -\eta \nabla_{\theta} \ell(\theta_k) + \eta C(\theta_k) W_{k+1}, \quad W_k \sim \mathcal{N}(0, I), \text{ i.i.d.}$$

is a order 1 strong approximation to SDE (68)

$$d\Theta_t = -\nabla_{\theta} \ell(\Theta_t) dt + \sqrt{\eta} C(\Theta_t) dW_t, \quad \Theta_0 = \theta_0, \quad W_t \in \mathbb{R}^N \text{ is a standard Brownian motion (68)}$$

i.e., there exist a constant $C$ independent on $\eta$ but depending on $L$ and $M$ such that

$$E\|\Theta_{k\eta} - \theta_k\|^2 \leq C\eta^2, \quad \text{for all } 0 \leq k \leq \lfloor T/\eta \rfloor.$$

Proof. We show that, as $\eta \to 0$, the discrete iteration $\theta_k$ of Eq. (67) in strong norm and on finite–time intervals is close to the solution of the SDE (68). The main techniques follow [3], but [3] only considered the case when $C(\theta)$ is a constant.

For vector $x \in \mathbb{R}^d$, we define its norm as $|x| := \sqrt{x^T x}$; for matrix $X \in \mathbb{R}^{d_1 \times d_2}$, we define its norm as $|X| := \sqrt{\text{Tr}(X^T X)} = \sqrt{\text{Tr}(XX^T)}$.

Let $\hat{\Theta}_t$ be the process defined by the integral form of the stochastic differential equation

$$\hat{\Theta}_t - \hat{\Theta}_0 = -\int_0^t \nabla_{\theta} \ell(\hat{\Theta}_{s\eta}) ds + \sqrt{\eta} \int_0^t C(\hat{\Theta}_{s\eta}) dW_s, \quad \hat{\Theta}_0 = \theta_0.$$

Hence the inequality holds.

A.4 Proof of Theorem 3

Theorem. (Rigorous statement of Theorem 3: Strong convergence between M-SGD-Gaussian and SDE) Let $T \geq 0$. Let $C(\theta)$ be the diffusion matrix, e.g., $C(\theta) = \frac{\sqrt{DB}C(\Theta)}{\sqrt{N}} \in \mathbb{R}^{D \times N}$. Assume there exist some $L, M > 0$ such that $\max_{i=1,2,...,N} \max_{x} (|\nabla \ell_i(x)|) \leq M$ and that $\nabla \ell_i(x)$ are Lipschitz continuous with bounded Lipschitz constant $L > 0$ uniformly for all $i = 1, 2, ..., N$.

Then the M-SGD-Gaussian iteration (67)

$$\theta_{k+1} - \theta_k = -\eta \nabla_{\theta} \ell(\theta_k) + \eta C(\theta_k) W_{k+1}, \quad W_k \sim \mathcal{N}(0, I), \text{ i.i.d.}$$

is a order 1 strong approximation to SDE (68)

$$d\Theta_t = -\nabla_{\theta} \ell(\Theta_t) dt + \sqrt{\eta} C(\Theta_t) dW_t, \quad \Theta_0 = \theta_0, \quad W_t \in \mathbb{R}^N \text{ is a standard Brownian motion (68)}$$

i.e., there exist a constant $C$ independent on $\eta$ but depending on $L$ and $M$ such that

$$E\|\Theta_{k\eta} - \theta_k\|^2 \leq C\eta^2, \quad \text{for all } 0 \leq k \leq \lfloor T/\eta \rfloor.$$

Proof. We show that, as $\eta \to 0$, the discrete iteration $\theta_k$ of Eq. (67) in strong norm and on finite–time intervals is close to the solution of the SDE (68). The main techniques follow [3], but [3] only considered the case when $C(\theta)$ is a constant.

For vector $x \in \mathbb{R}^d$, we define its norm as $|x| := \sqrt{x^T x}$; for matrix $X \in \mathbb{R}^{d_1 \times d_2}$, we define its norm as $|X| := \sqrt{\text{Tr}(X^T X)} = \sqrt{\text{Tr}(XX^T)}$.

Let $\hat{\Theta}_t$ be the process defined by the integral form of the stochastic differential equation

$$\hat{\Theta}_t - \hat{\Theta}_0 = -\int_0^t \nabla_{\theta} \ell(\hat{\Theta}_{s\eta}) ds + \sqrt{\eta} \int_0^t C(\hat{\Theta}_{s\eta}) dW_s, \quad \hat{\Theta}_0 = \theta_0.$$
We first bound

\[ \hat{\Theta}_{k+1} - \hat{\Theta}_k = -\eta \nabla_\theta L(\hat{\Theta}_k) - \sqrt{\eta} C(\hat{\Theta}_k)(W_{k+1} - W_k) . \]  

(71)

Since \( \sqrt{\eta}(W_{k+1} - W_k) \sim \mathcal{N}(0, \eta^2 I) \), we could let \( \eta W_{k+1} = \sqrt{\eta}(W_{k+1} - W_k) \), where \( W_{k+1} \) is the i.i.d. Gaussian sequence in (67). From here, we see that

\[ \hat{\Theta}_k = \theta_k , \]  

(72)

where \( \theta_k \) is the solution to (67).

We first bound \( \hat{\Theta}_t \) in Eq. (70) and \( \Theta_t \) in Eq. (68). Then we could obtain the error estimation of \( \theta_k = \hat{\Theta}_k \) and \( \Theta_k \) by simply set \( t = k \).

Since we assumed that \( \nabla_\theta \ell_i(\theta) \) is \( L \)-Lipschitz continuous, we get

\[ |C(\theta_1) - C(\theta_2)| = \frac{1}{\sqrt{bN}} \sqrt{\sum_{i=1}^{N} |\nabla_\theta \ell_i(\theta_1) - \nabla_\theta \ell_i(\theta_2)|^2} \leq \frac{1}{\sqrt{bN}} \sqrt{NL^2|\theta_1 - \theta_2|^2} \leq L|\theta_1 - \theta_2| \text{ since } b \geq 1 . \]

Thus \( C(\theta) \) is also \( L \)-Lipschitz continuous. Take a difference between (70) and (68) we get

\[ \hat{\Theta}_t - \Theta_t = -\int_0^t [\nabla_\theta L(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)] \, ds + \sqrt{\eta} \int_0^t [C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)] \, dW_s . \]  

(73)

We can estimate

\[ |\nabla_\theta L(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)|^2 \]

\[ \leq 2|\nabla_\theta L(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_{\lfloor \frac{s}{h} \rfloor})|^2 + 2|\nabla_\theta L(\Theta_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)|^2 \]

\[ \leq 2L^2|\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor} - \Theta_{\lfloor \frac{s}{h} \rfloor}|^2 + 2L^2|\Theta_{\lfloor \frac{s}{h} \rfloor} - \Theta_s|^2 , \]

(74)

where we used the inequality \( |\nabla_\theta L(\theta_1) - \nabla_\theta L(\theta_2)| \leq \frac{1}{N} \sum_{i=1}^{N} |\nabla_\theta \ell_i(\theta_1) - \nabla_\theta \ell_i(\theta_2)| \leq L|\theta_1 - \theta_2| \).

Similarly, we estimate

\[ |C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)|^2 \]

\[ \leq 2|C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_{\lfloor \frac{s}{h} \rfloor})|^2 + 2|C(\Theta_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)|^2 \]

\[ \leq 2L^2|\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor} - \Theta_{\lfloor \frac{s}{h} \rfloor}|^2 + 2L^2|\Theta_{\lfloor \frac{s}{h} \rfloor} - \Theta_s|^2 . \]

(75)

On the other hand, from (73), the Itô’s isometry (23) and Cauchy–Schwarz inequality we have

\[ \mathbb{E}|\hat{\Theta}_t - \Theta_t|^2 \]

\[ \leq 2\mathbb{E} \int_0^t |\nabla_\theta L(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)|^2 \, ds + 2\eta \mathbb{E} \int_0^t |C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)|^2 \, dW_s \]

\[ \leq 2\mathbb{E} \int_0^t |\nabla_\theta L(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)|^2 \, ds + 2\eta \int_0^t \mathbb{E} |C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)|^2 \, ds \]

\[ \leq 2\mathbb{E} \int_0^t |\nabla_\theta L(\Theta_{\lfloor \frac{s}{h} \rfloor}) - \nabla_\theta L(\Theta_s)|^2 \, ds + 2\eta \int_0^t \mathbb{E} |C(\hat{\Theta}_{\lfloor \frac{s}{h} \rfloor}) - C(\Theta_s)|^2 \, ds . \]

(76)
Combining (74), (75) and (76) we obtain that
\[ E[\hat{\Theta}_t - \Theta_t|^2 \leq 2 \int_0^t \left( 2L^2 E[\hat{\Theta}_{(\xi,j)|\eta} - \Theta_{(\xi,j)|\eta}^2 + 2L^2 E[\hat{\Theta}_{(\xi,j)|\eta} - \Theta_s|^2 \right) ds \\
+ 2\eta \int_0^t \left( 2L^2 E[\hat{\Theta}_{(\xi,j)|\eta} - \Theta_{(\xi,j)|\eta}^2 + 2L^2 E[\hat{\Theta}_{(\xi,j)|\eta} - \Theta_s|^2 \right) ds . \]  
(77)

Since we assumed that there is an \( M > 0 \) such that \( \max_{i=1,2,...,N} (|\nabla_\theta L_i(\theta)|) \leq M \), we conclude that
\[ |\nabla_\theta L(t)| \leq \frac{1}{N} \sum_{i=1}^{N} |\nabla_\theta L_i(\theta)| \leq M \] and \( |C(\theta)| \leq \frac{1}{\sqrt{bN}} \sqrt{\sum_{i=1}^{N} |\nabla_\theta L_i(\theta)|^2} \leq M \) since \( b \geq 1 \). By (68), the Itô’s isometry, the Cauchy–Schwarz inequality and \( 0 \leq s - \lfloor \frac{\eta}{\theta} \rfloor \eta \leq \eta \) we know that
\[ E[\Theta_{(\xi,j)|\eta} - \Theta_s|^2 = E\left| - \int_{\lfloor \frac{\eta}{\theta} \rfloor \eta}^{s} \nabla_\theta L(\Theta_u) du + \sqrt{\eta} \int_{\lfloor \frac{\eta}{\theta} \rfloor \eta}^{s} C(\Theta_u) dW_u \right|^2 \leq 2E\left( \int_{\lfloor \frac{\eta}{\theta} \rfloor \eta}^{s} |\nabla_\theta L(\Theta_u)| du \right)^2 + 2\eta E\left( \int_{\lfloor \frac{\eta}{\theta} \rfloor \eta}^{s} C(\Theta_u) dW_u \right)^2 \leq 2\eta^2 M^2 + 6\eta^2 M^2 = 8\eta^2 M^2 . \]  
(78)

Combining (78) and (77) we obtain
\[ E[\hat{\Theta}_t - \Theta_t|^2 \leq 4(1 + \eta)L^2 \left( \int_0^t E[\hat{\Theta}_{(\xi,j)|\eta} - \Theta_{(\xi,j)|\eta}^2 ds + 4\eta^2 M^2 t \right) . \]  
(79)

Set \( T > 0 \) and \( m(t) = \max_{0 \leq s \leq t} E[\hat{\Theta}_s - \Theta_s|^2 \), noticing that \( m(\lfloor \frac{\eta}{\theta} \rfloor \eta) \leq m(s) \) (as \( \lfloor \frac{\eta}{\theta} \rfloor \eta \leq s \)), then the above gives for any \( 0 \leq t \leq T \),
\[ m(t) \leq 4(1 + \eta)L^2 \left( \int_0^t m(s) ds + 4\eta^2 M^2 T \right) . \]  
(80)

By Gronwall’s inequality we obtain that for \( 0 \leq t \leq T \),
\[ m(t) \leq 16(1 + \eta)L^2 \eta^2 M^2 T e^{4(1+\eta)L^2 t} . \]  
(81)

Suppose \( 0 < \eta < 1 \), then there is a constant \( C \) which is independent on \( \eta \) s.t.
\[ E[\hat{\Theta}_t - \Theta_t|^2 \leq m(t) \leq C\eta^2 . \]  
(82)

Set \( t = k\eta \) in (82) and make use of (72), we finish the proof.

\[ \square \]

**Remark.** As we have seen in the previous proof, the functions \( \nabla_\theta L(\theta) \) and \( C(\theta) \) are both \( L \)-Lipschitz continuous, and thus the SDE (68) admits a unique solution (23, Section 5.2).
B Experiments Setup and Further Results

The different algorithms are explained as follows:

- GD: vanilla GD.
- SGD: vanilla SGD.
- SGD-b: vanilla SGD with batch size $b$.
- M-SGD-Fisher: M-SGD-Gaussian, the covariance of Gaussian M-Noise is the empirical Fisher scaled by SGD batch size.
- M-SGD-Cov: M-SGD-Gaussian, the covariance of Gaussian M-Noise is the gradient covariance scaled by SGD batch size.
- GD-Rademacher: use vanilla GD to optimize loss with Rademacher regularizer. We approximately solve the Rademacher regularizer by abandoning the maximum operator and the absolute value operator. There is a hyper parameter to scale Rademacher regularizer, which is tuned to be optimal.
- M-SGD-[Fisher-b]: M-SGD-Gaussian, the covariance of Gaussian M-Noise is the estimated Fisher using only $b$ randomly sampled training data, instead of using all training data. We scale the covariance of the M-Noise to force it sharing the same scale with that of the M-Noise in M-SGD-Fisher.
- M-SGD-[Cov-b]: M-SGD-Gaussian, the covariance of Gaussian M-Noise if the estimated gradient covariance using only $b$ randomly sampled training data, instead of using all training data. We scale the covariance of the M-Noise to force it sharing the same scale with that of the M-Noise in M-SGD-Cov.
- [M-SGD-Fisher]-b: M-SGD-Gaussian, the M-Noise is a $b$-sparse Gaussian, i.e., it has at most $b$ non-zero values, and its covariance is the estimated Fisher using only $b$ training data. The sparse noise is generated by composing the procedure of sampling mini-batch and drawing Gaussian noise. We scale the covariance of the M-Noise to force it sharing the same scale with that of the M-Noise in M-SGD-Fisher.
- [M-SGD-Cov]-b: M-SGD-Gaussian, the M-Noise is a $b$-sparse Gaussian, i.e., it has at most $b$ non-zero values, and its covariance is the estimated gradient covariance using only $b$ training data. The sparse noise is generated by composing the procedure of sampling mini-batch and drawing Gaussian noise. We scale the covariance of the M-Noise to force it sharing the same scale with that of the M-Noise in M-SGD-Cov.

Remark that the M-Noises of M-SGD-[Fisher-b] and M-SGD-[Cov-b] do no have to be sparse, which are different from [M-SGD-Fisher]-b and [M-SGD-Cov]-b.

All the experiments are implemented by PyTorch 1.0.0. We will make code available for reproducibility.

B.1 FashionMNIST

Dataset We randomly choose 1,000 original test data as our training set, and 60,000 original training data as our test set. Thus we have 1,000 training data and 60,000 test data. The only pre-processing is scaling image into $[0, 1]$.

Model We use a LeNet like network:

$$
\text{input} \Rightarrow \text{conv1} \Rightarrow \text{max\_pool} \Rightarrow \text{ReLU} \Rightarrow \text{conv2} \Rightarrow \\
\text{max\_pool} \Rightarrow \text{ReLU} \Rightarrow \text{fc1} \Rightarrow \text{ReLU} \Rightarrow \text{fc2} \Rightarrow \text{output}.
$$

Both two convolutional layers use $5 \times 5$ kernels with 10 channels and no padding. The number of hidden units between fully connected layers are 50. The total number of parameters of this network are 11,330.

Optimization We use standard (stochastic) gradient descent optimizer. The learning rate is 0.01. If not stated otherwise, the batch size of SGD is 50.
Figure 2: (a)(b): CIFAR-10 trained on VGG-11 without BN. **M-SGD-Fisher**: M-SGD-Gaussian with Fisher as covariance; **M-SGD-Cov**: M-SGD-Gaussian with gradient as covariance; **M-SGD-Bernoulli**: M-SGD with Bernoulli M-Noise, which independent approximation of the M-Noise of SGD; **[M-SGD-Fisher]-b**: M-SGD with sparse M-Noise, which is the composition of a Bernoulli noise and a Gaussian noise with Fisher as covariance. **[M-SGD-Cov]-b**: named in the same spirit with [M-SGD-Fisher]-b. The covariance matrices of all M-Noises are scaled such that they are in the same scale with that of SGD.

Figure 3: (a)(b): CIFAR-10 trained on ResNet-11. We do not use data augmentation and weight decay. **M-SGD-Fisher**: M-SGD-Gaussian with Fisher as covariance; **M-SGD-Cov**: M-SGD-Gaussian with gradient as covariance; **M-SGD-Bernoulli**: M-SGD with Bernoulli M-Noise, which independent approximation of the M-Noise of SGD; **[M-SGD-Fisher]-b**: M-SGD with sparse M-Noise, which is the composition of a Bernoulli noise and a Gaussian noise with Fisher as covariance. **[M-SGD-Cov]-b**: named in the same spirit with [M-SGD-Fisher]-b. The covariance matrices of all M-Noises are scaled such that they are in the same scale with that of SGD.

B.2 SVHN

**Dataset** We randomly choose 25,000 original test data as our training set, and 75,000 original training data as our test set. Thus we have 25,000 training data and 75,000 test data. The only pre-processing is scaling image into $[0, 1]$.

**Model** We use standard VGG-11 without Batch Normalization, for the purpose of eliminating the noise introduced by Batch Normalization.

**Optimization** We use standard (stochastic) gradient descent optimizer. The learning rate is 0.05. If not stated otherwise, the batch size of SGD is 100.

B.3 CIFAR-10

**Dataset** We use standard CIFAR-10 dataset. We scale the image into $[0, 1]$. 

Models  We use two models: standard VGG-11 without Batch Normalization and standard ResNet-18 with (Batch Normalization). For the training of ResNet-18, we adopt Ghost Batch Normalization [11] to eliminate the noise introduced by Batch Normalization with different batch size.

Optimization for VGG-11  We use momentum (stochastic) gradient descent optimizer. The momentum is 0.9. The learning rate is 0.01 decayed by 0.1 at iteration 40,000 and 60,000. If not stated otherwise, the batch size of SGD is 100.

Optimization for ResNet-18  We use momentum (stochastic) gradient descent optimizer. The momentum is 0.9. The learning rate is 0.1 decayed by 0.1 at iteration 40,000 and 60,000. If not stated otherwise, the batch size of SGD is 100.

Specially, for the experiments to obtain state-of-the-art performance on ResNet-18, we also use standard data augmentation and weight decay $5 \times 10^{-4}$.

More results  Figure 2 and Figure 3 provide additional experiment to validate our understanding in main paper. Our experiments are consistent with the ones in main paper.