Limiting fluctuation of multilayer neural networks with mean field training

Abstract

The mean field theory of multilayer neural networks centers around a particular infinite-width scaling, in which the learning dynamics is shown to be closely tracked by the mean field limit. A random fluctuation around this infinite-width limit is expected from a large-width expansion to the next order. This fluctuation has been studied only in the case of shallow networks, where previous works employ heavily technical notions or additional formulation ideas amenable only to that case. Treatment of the multilayer case has been missing, with the chief difficulty in finding a formulation that must capture the stochastic dependency across not only time but also depth.

In this work, we initiate the study of the fluctuation in the case of multilayer networks, at any network depth. Leveraging on the neuronal embedding framework recently introduced in Nguyen and Pham 2020 [13], we systematically derive a system of dynamical equations, called the *second-order mean field limit*, that captures the limiting fluctuation distribution. We demonstrate through the framework the complex interaction among neurons in this second-order mean field limit, the stochasticity with cross-layer dependency and nonlinear time evolution inherent in the limiting fluctuation. A limit theorem is proven to relate quantitatively this limit to the fluctuation realized by large-width networks.

We then apply the result to show that in the large-width regime, gradient descent training helps reducing and eventually eliminating the variance of the learned output function, provided the learning dynamics converges sufficiently fast to (or is initialized at) a global optimum. This extends a similar phenomenon previously shown only for shallow networks with a squared loss in the empirical risk minimization setting, to multilayer networks with a loss function that is not necessarily convex in a more general setting.

1 Introduction

Recent literature has witnessed much interest and progresses in the mean field theory of neural networks. In particular, it is shown that under a suitable scaling, as the widths tend to infinity, the neural network's learning dynamics converges to a nonlinear deterministic limit, known as the mean field (MF) limit [10, 13]. This line of works starts with analyses of the shallow case under various settings and has led to a number of nontrivial exciting results [14, 10, 5, 18, 20, 7, 17, 15, 24, 19, 25, 9, 1, 12]. The generalization to multilayer neural networks, already much more conceptually and technically challenging, has also been met with serious efforts from different groups of authors, with various novel ideas and insights [11, 13, 16, 2, 21, 6].

Since the MF limit is basically a first-order infinite-width approximation of the neural network, it is natural to consider the next order term in the expansion for a more faithful finite-width description.

This leads to the consideration of the fluctuation, up-scaled appropriately with the widths, around the MF limit. On one hand, this fluctuation should display MF interactions among neurons. On the other hand, it is random due to the inherent stochasticity in the finite-width network which, for instance, is randomly initialized and hence induces randomness in the interactions among neurons.

For shallow networks, [22, 18, 3] has identified the limiting fluctuation in the form of a time-evolving signed measure over weights, leading to a central limit theorem (CLT) in the space of measures. In particular, [22] pinpoints the fluctuation via a compactness argument in an appropriate measure space. Avoiding the heavy technicality, [3] realizes a neat trick, specific to shallow networks, where quantities of interest are described via push-forward of the initialized values of the weights.

There has been no similar attempt for the multilayer case, which faces major obstacles in formulating the limiting fluctuation. Firstly, existing formulations of the MF limit already move away from working with measures over weights [11, 13, 21, 6], unless restricted conditions are assumed [2]. This is due to the complexity of MF interactions: the presence of middle layers brings about simultaneous actions of multiple symmetry groups. We face the same complexity when formulating the fluctuation. Secondly, unlike shallow networks, the fluctuation in multilayer networks displays stochastic dependency not only through time but also across layers. Specifically the cross-layer dependency is propagated by both forward and backward propagation signals, at any time instance.

Contributions. We tackle the challenge by leveraging on the neuronal embedding framework, recently proposed by [13]. An important concept that is supported by the neuronal embedding is the sampling of neurons. We use this concept to formulate the limiting fluctuation via a decomposition into two components with different roles. One component is a random process, which encodes CLT-like stochasticity in the fluctuation of the sampled neurons around the MF ensemble. The other component, named the *second-order mean field limit*, is a system of ODEs, which displays MF interactions in the deviation of the neural network under GD training from the sampled neurons.

This decomposition is an innovation of the work. Our formulation enjoys the generality brought about by the neuronal embedding framework without restrictive assumptions (e.g. i.i.d. initialization assumption made in [2, 21]) and faithfully describes the expected stochastic dependency across time and depth. We prove a limit theorem that establishes the connection with the fluctuation in finite-sized networks. Unlike [22, 3], this result is quantitative.

Using this formulation, we show that gradient descent (GD) in a large-width multilayer network has a variance reduction effect: the (width-corrected) variance of the learned output function is shown to be non-increasing with time and eventually vanish. This holds even if the network is initialized at, or if it is trained to converge sufficiently fast to, a global optimum. This phenomenon has been shown in the shallow case [3], which requires a squared loss in the empirical risk minimization setup. As demonstrated by our result, it is not an isolated phenomenon and can indeed hold for a neural architecture where MF interactions are more complex, a loss function that is not necessarily convex and a training setup unrestricted to finitely many training data points.

Limitations and potential extensions. Let us finally mention a few limitations. Our work considers fully-connected multilayer networks trained with GD, a setup much less general than [13]. We expect certain extensions in this direction are doable. We also do not treat stochastic GD and hence disregard the stochasticity of data sampling, unlike [22]. Given the broader literature on this subject (e.g. [8]), this extension is foreseeable. Here we focus instead on the stochasticity that is inherent in the interactions among neurons, which is the more interesting aspect of neural networks.

Our result on the output variance is specific to unregularized training, unlike [3], and also requires a sufficient global convergence rate. While there have been several proven global convergence guarantees for multilayer networks [13, 16], understanding of the convergence rate is still lacking. Even in the shallow case, global convergence has been studied only for a type of sparsity-inducing regularization [5, 4]. Unless the convergence rate for multilayer networks is generally perilous (an unlikely scenario in light of the experiments in [11]), our result is expected to be relevant.

Notations. We use K to denote a generic constant that may change from line to line, and similarly K_u for a finite constant that may depend on some constant u. For simplicity, for L the network depth, we write K in place of K_L. For $\mathbb{E}$ (resp. $\mathbf{E}$) being the expectation, we use $\mathbb{V}$ and $\mathbb{C}$ (resp. $\mathbf{V}$ and $\mathbf{C}$) for the variance and covariance. We write $\mathbb{E}_Z$ for the expectation w.r.t. data $Z = (X, Y) \sim \mathcal{P}$.

2 Background on the MF limit for multilayer networks and assumptions

We describe the necessary backgrounds based on (and simplifying) the work [13]. This section also introduces several important notations, as well as the assumptions for our study of the fluctuation.

Multilayer network. Following [13], we consider a L-layer fully-connected neural network with widths $\{N_i\}_{i \leq L}$ (for $N_L = 1$):

$$\hat{\mathbf{y}}(t,x) = \varphi_L (\mathbf{H}_L (t,1,x)),$$

$$\mathbf{H}_i (t,j_i,x) = \mathbb{E}_{J_{i-1}} \left[\mathbf{w}_i (t,J_{i-1},j_i) \varphi_{i-1} (\mathbf{H}_{i-1} (t,J_{i-1},x)) \right], \qquad i = L,...,2,$$

$$\mathbf{H}_1 (t,j_1,x) = \langle \mathbf{w}_1 (t,1,j_1), x \rangle,$$

in which $x \in \mathbb{X} = \mathbb{R}^d$ is the input, the weights are $\mathbf{w}_1 (t,1,j_1) \in \mathbb{W}_1 = \mathbb{R}^d$ and $\mathbf{w}_i (t,j_{i-1},j_i) \in \mathbb{W}_i = \mathbb{R}$, $\varphi_i : \mathbb{R} \to \mathbb{R}$ is the activation and $t \in \mathbb{T} = \mathbb{R}_{\geq 0}$ the continuous time. Here we reserve the notation J_i for the random variable $J_i \sim \text{Unif}([N_i])$ and we write $\mathbb{E}_J$ to denote the expectation w.r.t. these random variables. For convenience, we take $j_0 \in \{1\}$ and $N_0 = 1$.

We train the network with gradient descent (GD) w.r.t. the loss $\mathcal{L} : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_{\geq 0}$ and the data $Z = (X,Y) \in \mathbb{X} \times \mathbb{R}$ drawn from a training distribution $\mathcal{P}$. Given an initialization $\mathbf{w}_i (0,\cdot,\cdot)$, we perform the update:

$$\partial_t \mathbf{w}_i (t,j_{i-1},j_i) = -\mathbb{E}_Z \left[\partial_2 \mathcal{L} (Y,\hat{\mathbf{y}}(t,X)) \frac{\partial \hat{\mathbf{y}}(t,X)}{\partial \mathbf{w}_i (j_{i-1},j_i)} \right], \quad i \in [L], \ j_i \in [n_i], \ j_{i-1} \in [n_{i-1}],$$

in which we define

$$\frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{H}_i (j_i)} = \begin{cases} \varphi_L' (\mathbf{H}_L (t,1,x)), & i = L, \\ \mathbb{E}_{J_{i+1}} \left[\frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{H}_{i+1} (J_{i+1})} \mathbf{w}_{i+1} (t,j_i,J_{i+1}) \varphi_i' (\mathbf{H}_i (t,j_i,x)) \right], & i < L, \end{cases}$$

$$\frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{w}_i (j_{i-1},j_i)} = \begin{cases} \frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{H}_i (j_i)} \varphi_{i-1} (\mathbf{H}_{i-1} (t,j_{i-1},x)), & i > 1, \\ \frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{H}_1 (j_1)} x, & i = 1. \end{cases}$$

One may recognize that these "derivative" quantities are defined in a perturbative fashion; for instance, $\frac{\partial \hat{\mathbf{y}}(t,x)}{\partial \mathbf{H}_i(j_i)}$ represents how much $\hat{\mathbf{y}}(t,x)$ changes (rescaled by widths) as one perturbs $\mathbf{H}_i (t,j_i,x)$.

Mean field limit. The MF limit is defined upon a given neuronal ensemble $(\Omega, \mathcal{F}, P) = \prod_{i=0}^{L} (\Omega_i, \mathcal{F}_i, P_i)$ (in which $\Omega_0 = \Omega_L = \{1\}$), which is a product probability space. We reserve the notation C_i for the random variable $C_i \sim P_i$ and we write $\mathbb{E}_C$ to denote the expectation w.r.t. these random variables. The MF limit that is associated with the network (1) is described by the evolution of $\{w_i (t,\cdot,\cdot)\}_{i \in [L]}$, given by the following MF ODEs:

$$\partial_t w_i (t,c_{i-1},c_i) = -\mathbb{E}_Z \left[\partial_2 \mathcal{L} (Y,\hat{y}(t,X)) \frac{\partial \hat{y}(t,X)}{\partial w_i (c_{i-1},c_i)} \right], \quad i \in [L], \ c_i \in \Omega_i, \ c_{i-1} \in \Omega_{i-1},$$

where $w_i : \mathbb{T} \times \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i$ and $t \in \mathbb{T}$. Here we define the forward quantities:

$$\hat{y}(t,x) = \varphi_L (H_L (t,1,x)),$$

$$H_i (t,c_i,x) = \mathbb{E}_{C_{i-1}} \left[w_i (t,C_{i-1},c_i) \varphi_{i-1} (H_{i-1} (t,C_{i-1},x)) \right], \qquad i = L,...,2,$$

$$H_1 (t,c_1,x) = \langle w_1 (t,c_1), x \rangle,$$

and the backward quantities:

$$\frac{\partial \hat{y}(t,x)}{\partial H_i (c_i)} = \begin{cases} \varphi_L' (H_L (t,1,x)), & i = L, \\ \mathbb{E}_{C_{i+1}} \left[\frac{\partial \hat{y}(t,x)}{\partial H_{i+1} (C_{i+1})} w_{i+1} (t,c_i,C_{i+1}) \varphi_i' (H_i (t,c_i,x)) \right], & i < L, \end{cases}$$

$$\frac{\partial \hat{y}(t,x)}{\partial w_i (c_{i-1},c_i)} = \begin{cases} \frac{\partial \hat{y}(t,x)}{\partial H_i (c_i)} \varphi_{i-1} (H_{i-1} (t,c_{i-1},x)), & i > 1, \\ \frac{\partial \hat{y}(t,x)}{\partial H_1 (c_1)} x, & i = 1. \end{cases}$$

The evolution with time t of the MF limit is generally complex due to the nonlinear activations.

Sampling of neurons, neuronal embedding, and the neural net-MF limit connection. We describe the neuron sampling procedure that formalizes the connection between the MF limit and the neural network [13]. In particular, we independently sample $\{C_i(j_i)\}_{j_i \in [N_i]} \sim_{\text{i.i.d.}} P_i$ for $i = 1, ..., L$. Let us use $\mathbf{E}$ to denote the expectation w.r.t. the sampling randomness. Although [13] considers more general sampling rule, this suffices for our purposes.

Suppose that we are given initialization functions $w_i^0 : \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i$ and set the initializations for the neural network and the MF limit:

$$\mathbf{w}_i(0, j_{i-1}, j_i) = w_i^0(C_{i-1}(j_{i-1}), C_i(j_i)), \quad w_i(0, \cdot, \cdot) = w_i^0(\cdot, \cdot) \quad \forall i \in [L].$$

Then one lets the neural network and the MF limit to evolve according to their respective dynamics. The sampling of neurons hence allows to couple them and establish their connection on the basis of the tuple $(\Omega, \mathcal{F}, P, \{w_i^0\}_{i \in [L]})$ – known as *the neuronal embedding*, the key idea in [13].

[13] shows the following result. For any finite terminal time $T \in \mathbb{T}$, we have [1]:

$$\max_{i \in [L]} \mathbb{E}_J \left[\sup_{t \le T} |\mathbf{w}_i(t, J_{i-1}, J_i) - w_i(t, C_{i-1}(J_{i-1}), C_i(J_i))|^2 \right]^{1/2} = \tilde{O}(N_{\min}^{-c_*}) \tag{2}$$

with high probability, where $c_* > 0$ is a universal constant, $N_{\min} = \min_{i \in [L-1]} N_i$, $N_{\max} = \max_{i \in [L]} N_i$ and $\tilde{O}$ hides the dependency on T, L and $\log N_{\max}$. This result is fundamental and gives a useful suggestion that is to study the neural network via analyzing the MF limit. For example, [13] uses it to study the optimization efficiency of the neural network.

The sampling of neurons is inspired by the propagation of chaos argument [23], but is not a mere proof device. Indeed, in this work, we again make a crucial use of this sampling in the formulation of the limiting fluctuation (Section 3.3).

Set of assumptions. We consider the following assumptions for the rest of the paper:

Assumption 1. *We make the following assumptions:*

• *(Regularity)* φ_i *is K-bounded for $i \in [L-1]$, φ_i' and φ_i'' are K-bounded and K-Lipschitz for $i \in [L]$, $\partial_2 \mathcal{L}$ and $\partial_2^2 \mathcal{L}$ are K-bounded and K-Lipschitz in the second variable, and $|X| \le K$ almost surely.*

• *(Sub-Gaussian initialization)* $\sup_{m \ge 1} m^{-1/2} \mathbb{E}_C \left[|w_i^0(C_{i-1}, C_i)|^m \right]^{1/m} \le K$ *for any $i \in [L]$.*

• *(Measurability)* $L^2(P_i)$ *is separable for any $i \in [L]$.*

• *(Constant hidden widths)* $N_1 = ... = N_{L-1} = N$ *(with ideally $N \to \infty$).*

An example for the regularity assumption is $\varphi_L(u) = u$ the identity, $\varphi_i = \tanh$ for $i \in [L-1]$ and $\mathcal{L}(u_1, u_2)$ is a smooth version of the Huber loss. It is noteworthy that $\mathcal{L}$ does not need to be convex. The initialization assumption is also mild. These assumptions satisfy the conditions in the work [13]. Measurability assumption is a technical condition needed for well-defined-ness of the fluctuation; it is not conceptually restrictive and can accommodate results in [13].

The constant width assumption aligns with our interest in the infinite-width regime. Our development can be extended easily to the proportional scaling, where $N_i = \lfloor \rho_i N \rfloor$ for some constants $\rho_1, ..., \rho_{L-1} > 0$ with $N \to \infty$. These scalings are relevant to practical setups and also to yield interesting results. Specifically once some widths are much larger than others, we expect the fluctuation to be dominated by a subset of layers.

3 Limit system for the fluctuation around the MF limit

We describe our formulation for the fluctuation. As introduced, it is composed of two components: a stochastic process that induces Gaussian CLT-like behavior, and another process – called the second-order MF limit – that signifies the MF interactions at the fluctuation level. This is done on the basis of the sampling of neurons, on top of the neuronal embedding, introduced in Section 2.

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[1] While [13] treats stochastic GD in discrete time, this result is implicit in the proof.

We introduce the first component in Section 3.1 and then the second-oder MF limit in 3.2. Together the two components are connected with the fluctuation around the MF limit realized by a large-width network in Section 3.3, to give firstly the analog of (2) and secondly a limit theorem on the fluctuation distribution.

We end with a discussion in Section 3.4. All proofs are deferred to the appendix.

3.1 Gaussian component $\tilde{G}$

Recall the sampling of neurons described in Section 2. Given the MF limit, we define the following random quantities:

$$\tilde{y}(t,x) = \varphi_L(\tilde{H}_L(t,1,x)),$$

$$\tilde{H}_i(t,c_i,x) = \mathbb{E}_{J_{i-1}}\left[w_i(t,C_{i-1}(J_{i-1}),c_i)\,\varphi_{i-1}(\tilde{H}_{i-1}(t,C_{i-1}(J_{i-1}),x))\right], \qquad i = L,...,2,$$

$$\tilde{H}_1(t,c_1,x) = \langle w_1(t,c_1),x \rangle,$$

$$\frac{\partial\tilde{y}(t,x)}{\partial\tilde{H}_i(c_i)} = \begin{cases} \varphi_L'(\tilde{H}_L(t,1,x)), & i = L, \\ \mathbb{E}_{J_{i+1}}\left[\dfrac{\partial\tilde{y}(t,x)}{\partial\tilde{H}_{i+1}(C_{i+1}(J_{i+1}))}w_{i+1}(t,c_i,C_{i+1}(J_{i+1}))\,\varphi_i'(\tilde{H}_i(t,c_i,x))\right], & i < L, \end{cases}$$

$$\frac{\partial\tilde{y}(t,x)}{\partial w_i(c_{i-1},c_i)} = \begin{cases} \dfrac{\partial\tilde{y}(t,x)}{\partial\tilde{H}_i(c_i)}\varphi_{i-1}(\tilde{H}_{i-1}(t,c_{i-1},x)), & i > 1, \\ \dfrac{\partial\tilde{y}(t,x)}{\partial\tilde{H}_1(c_1)}x, & i = 1. \end{cases}$$

These quantities are analogues of the forward and backward MF quantities, but with $\mathbb{E}_{C_i}$ being replaced by an empirical average over $\{C_i(j_i)\}_{j_i \in [N_i]}$.

Now we define

$$\tilde{G}^y(t,x) = \sqrt{N}\,(\tilde{y}(t,x) - \hat{y}(t,x)),$$

$$\tilde{G}_i^w(t,c_{i-1},c_i,x) = \sqrt{N}\left(\frac{\partial\tilde{y}(t,x)}{\partial w_i(c_{i-1},c_i)} - \frac{\partial\hat{y}(t,x)}{\partial w_i(c_{i-1},c_i)}\right), \quad i = 1,...,L,$$

and let $\tilde{G}$ denote the collection of these functions. Notice that the randomness of $\tilde{G}$ is induced by the samples $C_i(j_i)$; thus we write the expectation w.r.t. $\tilde{G}$ via $\mathbf{E}$. Intuitively $\tilde{G}$ is the fluctuation of the sampled neurons around the MF limit and thus should converge to a Gaussian process. We show that this is indeed the case in the following mode of convergence.

Definition 1. Given joint distributions over a sequence (in N) of functions $\tilde{G}_{i,N} : \mathbb{T} \times \Omega_{i-1} \times \Omega_i \times \mathbb{X} \to \mathbb{W}_i$ for $i \in [L]$, we say that $\tilde{G}_N = \{\tilde{G}_{i,N}\}_{i \in [L]}$ *converges G-polynomially in moment* (as $N \to \infty$) to $\underline{G}$ if for any finite collection in ℓ of square-integrable $f_\ell : \mathbb{T} \times \Omega_{i(\ell)-1} \times \Omega_{i(\ell)} \times \mathbb{X} \to \mathbb{W}_{i(\ell)}$ that is continuous in time and integers $\alpha_\ell, \beta_\ell \geq 1$,

$$\sup_{t(\ell) \leq T\,\forall\ell}\left|\mathbb{E}\left[\prod_\ell\langle f_\ell, \tilde{G}_{i(\ell),N}^{\alpha_\ell}\rangle_{t(\ell)}^{\beta_\ell}\right] - \mathbb{E}\left[\prod_\ell\langle f_\ell, \underline{G}_{i(\ell)}^{\alpha_\ell}\rangle_{t(\ell)}^{\beta_\ell}\right]\right| = O_{D,T}\left(\sup_{t \leq T}\max_\ell\|f_\ell\|_t^D\right)/\sqrt{N},$$

for $D = \sum_\ell \alpha_\ell\beta_\ell$ and a constant terminal time T. Here we define:

$$\langle f,h\rangle_t = \mathbb{E}_{Z,C}\left[f(t,C_{i-1},C_i,X)\,h(t,C_{i-1},C_i,X)\right]$$

for any two such functions f and h, and $\|f\|_t^2 = \langle f,f\rangle_t$. As a convenient convention, if $f : \mathbb{T} \times \Omega_0 \times \Omega_1 \times \mathbb{X} \to \mathbb{W}_1$ is tested against $\tilde{G}_{1,N}$, we define $\langle f, \tilde{G}_{1,N}\rangle_t$ and $\|f\|_t$ using Euclidean inner product and the Euclidean norm.

Note that this mode of convergence gives a quantitative rate in N.

Theorem 2 (Gaussian component $\tilde{G}$). *For any terminal time $T \geq 0$, $\tilde{G}$ converges G-polynomially in moment to $\underline{G} = \{\underline{G}^y,\ \underline{G}_i^w,\ i \in [L]\}$, which is a collection of centered Gaussian processes.*

The covariance structure of $\underline{G}$ in Theorem 2 is explicit but lengthy; we refer to the appendix for full details. Here let us examine the variance of $\underline{G}^y$, given recursively by:

$$v_2(t,c_2,x) = \mathbb{V}_C\left[w_2(t,C_1,c_2)\,\varphi_1(H_1(t,C_1,x))\right],$$

$$v_i(t, c_i, x) = \mathbb{E}_C\big[\,|w_i(t, C_{i-1}, c_i)\,\varphi'_{i-1}(H_{i-1}(t, C_{i-1}, x))|^2\, v_{i-1}(t, C_{i-1}, x)\,\big]$$
$$+ \mathbb{V}_C\left[w_i(t, C_{i-1}, c_i)\,\varphi_{i-1}(H_{i-1}(t, C_{i-1}, x))\right], \quad i = 3, ..., L,$$
$$\mathbf{E}\big[\,|\underline{G}^y(t, x)|^2\,\big] = |\varphi'_L(H_L(t, 1, x))|^2\, v_L(t, 1, x)\,.$$

The recursive structure shows that $\underline{G}^y$ compounds the stochasticity propagated forwardly through the depth of the multilayer network. From the appendix, a similar observation can be made in the backward propagation direction.

3.2 Second-order MF limit

We introduce a system of ODE's for a dynamics that represents MF interactions at the fluctuation level. As we shall see later, this system gives a limiting description of the the deviation of the neural network from the sampled neurons under GD training.

Let us denote by G a collection of functions $G^y : \mathbb{T} \times \mathbb{X} \to \mathbb{R}$, $G_i^w : \mathbb{T} \times \Omega_{i-1} \times \Omega_i \times \mathbb{X} \to \mathbb{W}_i$ for $i \in [L]$, and let

$$\mathcal{G} = \{G : \|G\|_T < \infty \;\; \forall T \geq 0\}, \quad \|G\|_T = \sup_{t \leq T} \mathbb{E}_{Z,C}\Big[\,|G^y(t, X)|^2 + \sum_{i=1}^{L} |G_i^w(t, C_{i-1}, C_i, X)|^2\,\Big]^{1/2}.$$

We define processes $R_i : \mathcal{G} \times \mathbb{T} \times \Omega_{i-1} \times \Omega_i \to \mathbb{W}_i$ for $i \in [L]$ as follows. The processes R_i are initialized at $R_i(\cdot, 0, \cdot, \cdot) = 0$ for all i, and for each fixed $G \in \mathcal{G}$, solve the differential equations:

$$\partial_t R_i(G, t, c_{i-1}, c_i) =$$

$$- \mathbb{E}_Z\left[\frac{\partial \hat{y}(t, X)}{\partial w_i(c_{i-1}, c_i)} \partial_2^2 \mathcal{L}(Y, \hat{y}(t, X))\left(G^y(t, X) + \sum_{r=1}^{L} \mathbb{E}_C\left[R_r(G, t, C_{r-1}, C_r)\frac{\partial \hat{y}(t, X)}{\partial w_r(C_{r-1}, C_r)}\right]\right)\right]$$

$$- \mathbb{E}_Z\left[\partial_2 \mathcal{L}(Y, \hat{y}(t, X))\,\mathbb{E}_C\left[\sum_{r=1}^{L}\left[R_r(G, t, a, b)\frac{\partial^2 \hat{y}(t, X)}{\partial w_r(a, b)\,\partial w_i(c_{i-1}, c_i)}\right]_{a:=C_{r-1},\; b:=C_r}\right]\right]$$

$$- \mathbb{E}_Z\left[\partial_2 \mathcal{L}(Y, \hat{y}(t, X))\, G_i^w(t, c_{i-1}, c_i, X)\right]. \tag{3}$$

Here $\frac{\partial^2 \hat{y}(t,X)}{\partial w_r(a,b)\partial w_i(c_{i-1},c_i)}$ is defined in a perturbative fashion similar to those in Section 2 and is hence self-explanatory; we give the full explicit definitions in the appendix. We shall write $R_i(G, t) = R_i(G, t, \cdot, \cdot)$ for brevity. Let R denote the collection $\{R_i\}_{i \in [L]}$.

Theorem 3. *Under Assumption 1, for any $G \in \mathcal{G}$, there exists a unique solution $t \mapsto R_i(G, t, \cdot, \cdot) \in L^2(P_{i-1} \times P_i)$ which is continuous in time. Furthermore, for each t, $R(G, t)$ is a continuous linear functional in G.*

The process R is called the *second-order MF limit* for a reason we shall see shortly.

Remark 4. Care should be taken in the derivation of the "second derivative" quantity in Eq. (3). To illustrate, consider a simplified problem of taking a perturbation w.r.t. $w_r(a, b)$ of the quantity

$$g\left(w_i(c_{i-1}, c_i), \mathbb{E}_C\left[f_1(w_i(C_{i-1}, c_i))\right], \mathbb{E}_C\left[f_2(w_i(c_{i-1}, C_i))\right], \mathbb{E}_C\left[f_3(w_i(C_{i-1}, C_i))\right]\right) \equiv g(c_{i-1}, c_i).$$

For instance, when $r = i$, we have:

$$\left[R_i(G, t, a, b)\frac{\partial g(c_{i-1}, c_i)}{\partial w_r(a, b)}\right]_{a:=C_{i-1},\; b:=C_i}$$

$$= R_i(G, t, c_{i-1}, c_i)\,\partial_1 g(c_{i-1}, c_i) + R_i(G, t, C_{i-1}, c_i)\,\partial_2 g(c_{i-1}, c_i)\,\partial f_1(w_i(C_{i-1}, c_i))$$

$$+ R_i(G, t, c_{i-1}, C_i)\,\partial_3 g(c_{i-1}, c_i)\,\partial f_2(w_i(c_{i-1}, C_i)) + R_i(G, t, C_{i-1}, C_i)\,\partial_4 g(c_{i-1}, c_i)\,\partial f_3(w_i(C_{i-1}, C_i))\,.$$

3.3 Fluctuation around the MF limit via sampling of neurons

We are interested in a characterization of the following quantity, which represents the deviation of the weights of the neural network under GD training from the sampled neurons:

$$\mathbf{R}_i(t, j_{i-1}, j_i) = \sqrt{N}\left(\mathbf{w}_i(t, j_{i-1}, j_i) - w_i(t, C_{i-1}(j_{i-1}), C_i(j_i))\right).$$

Let $\mathbf{R}$ denote the collection $\{\mathbf{R}_i\}_{i \in [L]}$. We now state our first main result of the section.

Theorem 5 (Second-order MF)**.** *Under Assumption 1, we have, for any $t \leq T$,*

$$\mathbf{E}\mathbb{E}_J\left[\left|\mathbf{R}_i\left(t, J_{i-1}, J_i\right) - R_i(\tilde{G}, t, C_{i-1}\left(J_{i-1}\right), C_i\left(J_i\right))\right|^2\right] \leq K_T/N.$$

Upon the correct choice $\tilde{G}$, one deduces from the theorem the second-order expansion:

$$\mathbf{w}_i\left(t, j_{i-1}, j_i\right) \approx w_i\left(t, C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)\right) + N^{-1/2}R_i(\tilde{G}, t, C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)),$$

where the first-order term is directly from Eq. (2). As shall be seen from the derivation in Section 3.4, R characterizes the MF interactions among neurons at the fluctuation level, hence the name "second-order MF limit". Importantly this is done on the basis of the sampled neurons $\{C_i\left(j_i\right): j_i \in [N_i], i \in [L]\}$. Notably the dynamics of R_i at the i-th layer is dependent on all $\{R_k\}_{k \in [L]}$ and G^y, exemplifying the cross-layer interaction of fluctuations in multilayer networks.

Although Theorem 5 involves $\tilde{G}$, as shown in the derivation of Section 3.4, we actually do not utilize the specific structure of $\tilde{G}$. Incidentally we study the limiting structure of $\tilde{G}$ separately in Theorem 2. In other words, our decomposition of the fluctuation via $\tilde{G}$ and R allows relatively independent treatments of the two components of different natures, where one displays a CLT-like behavior and the other displays MF interactions.

Finally, combining the two theorems, we obtain the following CLT for the limiting output fluctuation.

Theorem 6 (CLT for output function)**.** *Under Assumption 1, the fluctuation $\sqrt{N}(\hat{\mathbf{y}}(t, x) - \hat{y}(t, x))$ converges weakly to the Gaussian process $\hat{G}$ indexed by $\mathbb{T} \times \mathbb{X}$:*

$$\hat{G}(t, x) = \sum_{i=1}^{L} \mathbb{E}_C\left[R_i(\underline{G}, t, C_{i-1}, C_i)\frac{\partial y(t, x)}{\partial w_i(C_{i-1}, C_i)}\right] + \underline{G}^y(t, x),$$

where $\underline{G}$ is the Gaussian process described in Theorem 2. Specifically, for any integer $m \geq 1$, $t \leq T$, and 1-bounded $h : \mathbb{X} \to \mathbb{R}$,

$$\left|\mathbf{E}\mathbb{E}_Z\left[h(X)\left(\sqrt{N}(\hat{\mathbf{y}}(t, X) - \hat{y}(t, X))\right)^m\right] - \mathbf{E}\mathbb{E}_Z\left[h(X)\left(\hat{G}(t, X)\right)^m\right]\right| \leq K_{T,m}/\sqrt{N}.$$

We note in passing the technicality we devise to prove Theorem 6. As noted, Theorems 5 and 2 separate treatments of R and $\tilde{G}$, but recall we are interested in $R(\tilde{G}, t)$. This necessitates a way to describe them jointly. We do so via the following notion of convergence, which extends the notion in Definition 1.

Definition 7. Suppose we are given a sequence (in N) of functions $\tilde{G}_{i,N} : \mathbb{T} \times \Omega_{i-1} \times \Omega_i \times \mathbb{X} \to \mathbb{W}_i$ for $i \in [L]$ such that $\tilde{G}_N = \{\tilde{G}_{i,N}\}_{i \in [L]}$ converges G-polynomially in moment to G. Given further $\tilde{R}_{i,N} : \mathbb{T} \times \Omega_{i-1} \times \Omega_i \times \mathbb{X} \to \mathbb{W}_i$ defined jointly with $\tilde{G}_{i,N}$ and $\tilde{R}_N = \{\tilde{R}_{i,N}\}_{i \in [L]}$, we say that $(\tilde{R}_N, \tilde{G}_N)$ *converges G-polynomially in moment and R-linearly in moment* (as $N \to \infty$) to (R, G) if for any f_ℓ, h_ℓ that are $\mathbb{T} \times \Omega_{i(\ell)-1} \times \Omega_{i(\ell)} \times \mathbb{X} \to \mathbb{W}_{i(\ell)}$ mappings and continuous in time and any integers $\alpha_\ell, \beta_\ell \geq 1$,

$$\sup_{t(\ell) \leq T \, \forall \ell}\left|\mathbb{E}\left[\prod_\ell\langle f_\ell, \tilde{G}_{i(\ell),N}^{\alpha_\ell}\rangle_{t(\ell)}^{\beta_\ell}\prod_\ell\langle h_\ell, \tilde{R}_{i(\ell),n}\rangle_{t(\ell)}^{\beta_\ell}\right] - \mathbb{E}\left[\prod_\ell\langle f_\ell, G_{i(\ell)}^{\alpha_\ell}\rangle_{t(\ell)}^{\beta_\ell}\prod_\ell\langle h_\ell, R_{i(\ell)}\rangle_{t(\ell)}^{\beta_\ell}\right]\right|$$
$$= O_D\left(\sup_{t \leq T}\max_\ell\|f_\ell\|_t^D, \sup_{t \leq T}\max_\ell\|h_\ell\|_t^D\right)/\sqrt{N},$$

for $D = \sum_\ell\beta_\ell\alpha_\ell + \sum_\ell\beta_\ell$.

Proposition 8. *Assume that $\tilde{G}$ converges G-polynomially in moment to $G = \{G^y, G_i^w, i \in [L]\}$. Then $(R(\tilde{G}, \cdot), \tilde{G})$ converges G-polynomially in moment and R-linearly in moment to $(R(G, \cdot), G)$.*

3.4 A heuristic derivation and discussion

A heuristic argument. We wish to give a heuristic to derive the relation between $\mathbf{R}_i$ and $R_i(\tilde{G}, t)$, i.e. Theorem 5. Suppose we look at the i-th layer:

$$\partial_t\mathbf{R}_i\left(t, j_{i-1}, j_i\right)$$

$$= \sqrt{N}\partial_t \mathbf{w}_i\left(t, j_{i-1}, j_i\right) - \sqrt{N}\partial_t w_i\left(t, C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)\right)$$

$$= \sqrt{N}\mathbb{E}_Z\left[\partial_2\mathcal{L}\left(Y, \hat{y}\left(t, X\right)\right)\frac{\partial \hat{y}\left(t, X\right)}{\partial w_i\left(C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)\right)}\right] - \sqrt{N}\mathbb{E}_Z\left[\partial_2\mathcal{L}\left(Y, \hat{\mathbf{y}}\left(t, X\right)\right)\frac{\partial \hat{\mathbf{y}}\left(t, X\right)}{\partial \mathbf{w}_i\left(j_{i-1}, j_i\right)}\right]$$

$$= \mathbb{E}_Z\left[\underbrace{\sqrt{N}\Big(\partial_2\mathcal{L}\left(Y, \hat{y}\left(t, X\right)\right) - \partial_2\mathcal{L}\left(Y, \hat{\mathbf{y}}\left(t, X\right)\right)\Big)}_{A_1} \cdot \frac{\partial \hat{y}\left(t, X\right)}{\partial w_i\left(C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)\right)}\right]$$

$$+ \mathbb{E}_Z\left[\partial_2\mathcal{L}\left(Y, \hat{\mathbf{y}}\left(t, X\right)\right) \cdot \sqrt{N}\left(\frac{\partial \hat{y}\left(t, X\right)}{\partial w_i\left(C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right)\right)} - \frac{\partial \hat{\mathbf{y}}\left(t, X\right)}{\partial \mathbf{w}_i\left(j_{i-1}, j_i\right)}\right)\right].$$

242   Let us zoom into A_1, with some care not to eliminate the fluctuation of interest:

$$A_1 \approx \sqrt{N}\partial_2^2\mathcal{L}\left(Y, \hat{y}\left(t, X\right)\right)\left(\hat{y}\left(t, X\right) - \hat{\mathbf{y}}\left(t, X\right)\right)$$

$$= \partial_2^2\mathcal{L}\left(Y, \hat{y}\left(t, X\right)\right)\left(-\tilde{G}^y\left(t, X\right) + \sqrt{N}\left(\tilde{y}\left(t, X\right) - \hat{\mathbf{y}}\left(t, X\right)\right)\right).$$

243   Now observe that $\tilde{y}\left(t, X\right) - \hat{\mathbf{y}}\left(t, X\right)$ is a difference between the sampled neurons and the neural
244 network, and hence one should be able to express it in terms of $\mathbf{R}$:

$$\sqrt{N}\left(\tilde{y}\left(t, X\right) - \hat{\mathbf{y}}\left(t, X\right)\right)$$

$$\approx \sum_{r=1}^L \mathbb{E}_J\left[\frac{\partial \tilde{y}\left(t, X\right)}{\partial w_r\left(C_{r-1}\left(J_{r-1}\right), C_r\left(J_r\right)\right)} \cdot \sqrt{N}\left(w_r\left(t, C_{r-1}\left(J_{r-1}\right), C_r\left(J_r\right)\right) - \mathbf{w}_r\left(t, J_{r-1}, J_r\right)\right)\right]$$

$$= -\sum_{r=1}^L \mathbb{E}_J\left[\frac{\partial \tilde{y}\left(t, X\right)}{\partial w_r\left(C_{r-1}\left(J_{r-1}\right), C_r\left(J_r\right)\right)} \cdot \mathbf{R}_r\left(t, J_{r-1}, J_r\right)\right].$$

245   Furthermore in the limit $N \to \infty$, we expect from the large of large numbers, for a test function f,

$$\mathbb{E}_J\left[f\left(C_{r-1}\left(J_{r-1}\right), C_r\left(J_r\right)\right)\right] \approx \mathbb{E}_C\left[f\left(C_{r-1}, C_r\right)\right]. \tag{4}$$

246 As such, one can identify the term that involves A_1 in the above equation for $\partial_t\mathbf{R}_i\left(t, j_{i-1}, j_i\right)$
247 with the first term in Eq. (3) for $\partial_t R_i\left(G, t, c_{i-1}, c_i\right)$. One can derive similarly for the rest of the
248 terms. With these, one arrives at $\partial_t\mathbf{R}_i\left(t, j_{i-1}, j_i\right) \approx \partial_t R_i(\tilde{G}, t, C_{i-1}\left(j_{i-1}\right), C_i\left(j_i\right))$. Recalling
249 that $\mathbf{R}_i\left(0, \cdot, \cdot\right) = 0 = R_i(\cdot, 0, \cdot, \cdot)$, one arrives at the conclusion of Theorem 5.

250   We see that the sampling of neurons makes transparent the derivation of R as the limit of $\mathbf{R}$: it
251 allows to compare one-to-one a "neuron" of the former to a neuron of the latter. This demonstrates
252 an advantage of the neuronal embedding framework, which easily accommodates the sampling of
253 neurons in the multilayer setup. We also see that the only involvement of $\tilde{G}$ in this derivation is via
254 its definition.

255 **Technical difficulties.** So far we have seen R captures the difference between the neural network
256 and the sampled neurons. Recall the other component in the fluctuation is the process $\tilde{G}$, which cap-
257 tures the $\sqrt{N}$-scaled difference between the sampled neurons and the MF limit. Taking into account
258 the whole system of fluctuation, we note a major technical subtlety: the aforementioned two differ-
259 ences captured by R and $\tilde{G}$ share the same source of randomness $\{C_i\left(j_i\right): \ j_i \in [N_i], \ i \in [L]\}$.

260   We mention two particular complications that arise from this subtlety. The first complication is how
261 one should define the process R in relation with $\tilde{G}$, given that R is meant to be the infinite-width
262 limit of $\mathbf{R}$ while $\mathbf{R}$ and $\tilde{G}$ are stochastically coupled. Our solution is to let $t \mapsto R(G, t)$ defined for
263 any $G \in \mathcal{G}$, not restricted to only $\tilde{G}$. This streamlines the definition of the second-order MF limit
264 and allows to separate our treatments of R and $\tilde{G}$, as evident from Theorems 5 and 2.

265   The second complication lies with Eq. (4). In fact, to arrive at the desired conclusion, we require the
266 function f to depend on $\tilde{G}$. This is because the main object of interest is $R(\tilde{G}, t)$, even though we
267 have treated R and $\tilde{G}$ separately. In a nutshell, f shares randomness with $C_r\left(j_r\right)$ and $C_{r-1}\left(j_{r-1}\right)$,
268 $j_r \in [N_r], j_{r-1} \in [N_{r-1}]$. The random variable on the left-hand side of Eq. (4) is therefore complex,
269 and it is highly questionable whether this equation should hold. The analysis becomes delicate;
270 without taking into account this shared randomness, the derivation would be a mere heuristic. As
271 we present in the proof, we verify this equation for a relevant set of functions f.

4 Asymptotic variance of the output function

We study the following width-scaled asymptotic variance quantity:

$$V^*(t) = \lim_{N \to \infty} \mathbf{E}\mathbb{E}_Z\left[\left|\sqrt{N}(\hat{\mathbf{y}}(t, X) - \hat{y}(t, X))\right|^2\right] = \lim_{N \to \infty} \mathbf{E}\mathbb{E}_Z\left[\left|\sqrt{N}(\hat{\mathbf{y}}(t, X) - \mathbf{E}[\hat{\mathbf{y}}(t, X)])\right|^2\right].$$

The second equality holds and the limits in N exist by Theorems 5 and 6. We make the following assumption.

Assumption 2. *We assume that* $\mathbb{E}_Z\left[\partial_2^2 \mathcal{L}(Y, f(X)) | X\right] = K$ *constant almost surely for any global optimizer f of* $\mathbb{E}_Z[\mathcal{L}(Y, f(X))]$.

Note that convexity of the loss is not required. This assumption is intuitive and in particular it holds for $\mathcal{L}(y, y') = \ell(y - y')$ for any quasi-convex smooth function ℓ, such as a smoothened Huber loss. Such a loss function is interesting: [13] shows that convergence to global optima is possible if either (case 1) $\mathcal{L}$ is convex in the second variable, or (case 2) $\partial_2 \mathcal{L}(y, y') = 0$ implies $\mathcal{L}(y, y') = 0$ (recalling $\mathcal{L} \geq 0$) and $Y = y(X)$ is a deterministic function of X. In both cases, one can find reasonable loss functions that satisfy Assumption 2. We also note that the situation in which the MF limit converges to a global optimum as $t \to \infty$ holds practical interests, and as such, it is desirable to further understand the evolution behavior of the fluctuation in such situation.

Our first result indicates that even if one initializes the network at a global optimum and hence there is no evolution with time at the MF limit level, GD training still helps by reducing the output variance $V^*(t)$ with time at the fluctuation level.

Theorem 9. *Suppose at initialization* $\mathbb{E}_Z[\partial_2 \mathcal{L}(Y, \hat{y}(0, X)) | X] = 0$ *a.s. Under Assumptions 1 and 2, $V^*(t)$ is non-increasing, and $V^*(t) \to 0$ as $t \to \infty$.*

This result suggests a variance-reduction effect of GD in the large-width regime. This continues to hold in the long-time horizon if, instead of initializing at a global optimum, we assume to have convergence at a sufficiently fast rate.

Theorem 10. *Assume* $\int_0^\infty t^{2+\delta} \mathbb{E}_X\left[|\mathbb{E}_Z[\partial_2 \mathcal{L}(Y, \hat{y}(t, X)) | X]|^2\right]^{1/2} dt < \infty$ *for some $\delta > 0$. Under Assumptions 1 and 2, $V^*(t) \to 0$ as $t \to \infty$.*

These results suggest that the variance reduction effect of GD in MF training is a phenomenon more general than the case of shallow networks with a squared loss and finitely many training points, previously treated in [3]. In particular, it is shown for multilayer networks with a loss function that is not necessarily convex with arbitrary training data distribution $\mathcal{P}$.

Let us briefly discuss the proof. For simplicity, consider the context of Theorem 9. Recall from Theorem 6 the Gaussian process $\hat{G}$ that the output fluctuation converges to as $N \to \infty$; we thus would like to show $\mathbf{E}\mathbb{E}_Z\left[|\hat{G}(t, X)|^2\right] \to 0$ as $t \to \infty$. In this case, one can show that for $\mathfrak{A}$: $L^2(\mathcal{P}) \to L^2(\mathcal{P})$ a linear operator defined by

$$(\mathfrak{A}f)(x) = -c \sum_i \mathbb{E}_{Z,C}\left[\frac{\partial \hat{y}(0, x)}{\partial w_i(C_{i-1}, C_i)} \frac{\partial \hat{y}(0, X)}{\partial w_i(C_{i-1}, C_i)} f(X)\right],$$

with a constant $c > 0$, we have $\partial_t \hat{G}(t, \cdot) = \mathfrak{A}\hat{G}(t, \cdot)$. In particular, $\mathfrak{A}$ is self-adjoint and has non-positive eigenvalues and as such, if at initialization $\hat{G}(0, \cdot)$ lies in the range of $\mathfrak{A}$, we reach the desired conclusion. This is simple in the shallow case. Indeed note that $\hat{G}(0, \cdot) = G^y(0, \cdot)$ by the assumption on initialization of Theorem 9. Assuming $\varphi_L(u) = u$ for simplicity, in the shallow case where $\hat{y}(0, x) = \mathbb{E}_{C_1}[w_2(0, C_1, 1) \varphi_1(\langle w_1(0, 1, C_1), x\rangle)]$, we have $G^y(0, \cdot)$ is zero-mean Gaussian with the covariance $\mathbf{E}[G^y(0, x) G^y(0, x')]$ equal to

$$\mathbb{C}_{C_1}[w_2(0, C_1, 1) \varphi_1(\langle w_1(0, 1, C_1), x\rangle); \; w_2(0, C_1, 1) \varphi_1(\langle w_1(0, 1, C_1), x'\rangle)].$$

Immediately from this simple covariance structure, we see that $x \mapsto G^y(0, x)$ lies in the span of $\{x \mapsto \varphi_1(\langle w_1(0, 1, c_1), x\rangle) : c_1 \in \text{supp}(P_1)\}$, i.e. the desired conclusion since $\frac{\partial \hat{y}(0, x)}{\partial w_2(C_1, 1)} = \varphi_1(\langle w_1(0, 1, C_1), x\rangle)$. In the multilayer case, this is no longer obvious due to the complex covariance structure as pointed out in Section 3, and yet interestingly we show that it still indeed holds.

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