Dynamical Mean Field Theory of Kernel Evolution in Wide Neural Networks

Blake Bordelon & Cengiz Pehlevan

John Paulson School of Engineering and Applied Sciences, Center for Brain Science
Harvard University
Cambridge MA, 02138
`blake_bordelon@g.harvard.edu, cpehlevan@g.harvard.edu`

Abstract

We analyze feature learning in infinite-width neural networks trained with gradient flow through a self-consistent dynamical field theory. We construct a collection of deterministic dynamical order parameters which are inner-product kernels for hidden unit activations and gradients in each layer at pairs of time points, providing a reduced description of network activity through training. These kernel order parameters collectively define the hidden layer activation distribution, the evolution of the neural tangent kernel, and consequently output predictions. We provide a sampling procedure to self-consistently solve for the kernel order parameters.

1   Introduction

Deep learning has emerged as a successful paradigm for solving challenging machine learning and computational problems across a variety of domains [1, 2]. However, theoretical understanding of the training and generalization of modern deep learning methods lags behind current practice. Ideally, a theory of deep learning would be analytically tractable, efficiently computable, capable of predicting network performance and internal features that the network learns, and interpretable through a reduced description involving desirably initialization-independent quantities.

Several recent theoretical advances have fruitfully considered the idealization of *wide neural networks*, where the number of hidden units in each layer is taken to be large. Under certain parameterization, Bayesian neural networks and gradient descent trained networks converge to gaussian processes (NNGPs) [3–5] and neural tangent kernel (NTK) machines [6–8] in their respective infinite-width limits. These limits provide both analytic tractability as well as detailed training and generalization analysis [9–16]. However, in this limit, with these parameterizations, data representations are fixed and do not adapt to data, termed the *lazy regime* of NN training, to contrast it from the *rich regime* where NNs significantly alter their internal features while fitting the data [17, 18]. The fact that the representation of data is fixed renders these kernel-based theories incapable of explaining feature learning, an ingredient which is crucial to the success of deep learning in practice [19, 20]. Thus, alternative theories capable of modeling feature learning dynamics are needed.

Recently developed alternative parameterizations such as the mean field [21] and the μP [22] parameterizations allow feature learning in infinite-width NNs trained with gradient descent. Using the Tensor Programs framework, Yang & Hu identified a stochastic process that describes the evolution of preactivation features in infinite-width μP NNs [22]. In this work, we study an equivalent parameterization to μP with self-consistent dynamical mean field theory (DMFT) and recover the stochastic process description of infinite NNs using this alternative technique. In the same large width scaling, we include a scalar parameter γ_0 that allows smooth interpolation between lazy and rich behavior [17]. We provide a new computational procedure to sample this stochastic process and demonstrate its predictive power for wide NNs.

The present work is a short version of our paper appearing in the main meeting [23]. Our contributions in these works are the following:

1. We develop a path integral formulation of gradient flow dynamics in infinite-width networks in the feature learning regime. Our parameterization includes a scalar parameter γ_0 to allow interpolation between rich and lazy regimes and comparison to perturbative methods.

2. Using a stationary action argument, we identify a set of saddle point equations that the kernels satisfy at infinite-width, relating the stochastic processes that define hidden activation evolution to the kernels and vice versa. We develop a numerical algorithm to solve these equations and show they are predictive of wide networks feature learning dynamics.

Our theory is inspired by self-consistent dynamical mean field theory (DMFT) from statistical physics [24–30]. This framework has been utilized in the theory of random recurrent networks [31–36], tensor PCA [37, 38], phase retrieval [39], and high-dimensional linear classifiers [40–43], but has yet to be developed for deep feature learning. By developing a self-consistent DMFT of deep NNs, we gain insight into how features evolve in the rich regime of network training, while retaining many pleasant analytic properties of the infinite-width limit.

2 Problem Setup and Definitions

Our theory applies to infinite-width networks, both fully-connected and convolutional. For notational ease we will focus on the MLP formalism. For input $\boldsymbol{x}_\mu \in \mathbb{R}^D$, we define the hidden *pre-activation* vectors $\boldsymbol{h}^\ell \in \mathbb{R}^N$ for layers $\ell \in \{1, ..., L\}$ as

$$f_\mu = \frac{1}{\gamma\sqrt{N}} \boldsymbol{w}^L \cdot \phi(\boldsymbol{h}_\mu^L) , \quad \boldsymbol{h}_\mu^{\ell+1} = \frac{1}{\sqrt{N}} \boldsymbol{W}^\ell \phi(\boldsymbol{h}_\mu^\ell) , \quad \boldsymbol{h}_\mu^1 = \frac{1}{\sqrt{D}} \boldsymbol{W}^0 \boldsymbol{x}_\mu, \tag{1}$$

where $\boldsymbol{\theta} = \mathrm{Vec}\{\boldsymbol{W}^0, ..., \boldsymbol{w}^L\}$ are the trainable parameters of the network and ϕ is a twice differentiable activation function. Inspired by previous works on the mechanisms of lazy gradient based training, the parameter γ will control the laziness or richness of the training dynamics [17, 18, 22, 44]. Each of the trainable parameters are initialized as Gaussian random variables with unit variance $W_{ij}^\ell \sim \mathcal{N}(0, 1)$. They evolve under gradient flow $\frac{d}{dt}\boldsymbol{\theta} = -\gamma^2 \nabla_{\boldsymbol{\theta}} \mathcal{L}$. The choice of learning rate γ^2 causes $\frac{d}{dt}\mathcal{L}|_{t=0}$ to be independent of γ. To characterize the evolution of weights, we introduce backpropagation variables $\boldsymbol{g}_\mu^\ell = \gamma\sqrt{N} \frac{\partial f_\mu}{\partial \boldsymbol{h}_\mu^\ell} = \dot{\phi}(\boldsymbol{h}_\mu^\ell) \odot \boldsymbol{z}_\mu^\ell$, where $\boldsymbol{z}_\mu^\ell = \frac{1}{\sqrt{N}} \boldsymbol{W}^{\ell\top} \boldsymbol{g}_\mu^{\ell+1}$ is the *pre-gradient* signal.

The relevant objects to characterize feature learning are feature and gradient kernels for each hidden layer $\ell \in \{1, ..., L\}$, defined as $\Phi_{\mu\alpha}^\ell(t, s) = \frac{1}{N}\phi(\boldsymbol{h}_\mu^\ell(t)) \cdot \phi(\boldsymbol{h}_\alpha^\ell(s))$, $G_{\mu\alpha}^\ell(t, s) = \frac{1}{N}\boldsymbol{g}_\mu^\ell(t) \cdot \boldsymbol{g}_\alpha^\ell(s)$. From these kernels $\{\Phi^\ell, G^\ell\}_{\ell=1}^L$, we can compute the *Neural Tangent Kernel* $K_{\mu\alpha}^{NTK}(t, s) = \nabla_{\boldsymbol{\theta}} f_\mu(t) \cdot \nabla_{\boldsymbol{\theta}} f_\alpha(s) = \sum_{\ell=0}^L G_{\mu\alpha}^{\ell+1}(t, s)\Phi_{\mu\alpha}^\ell(t, s)$, [6] and the dynamics of the network function f_μ

$$\frac{d}{dt} f_\mu(t) = \sum_{\alpha=1}^P K_{\mu\alpha}^{NTK}(t, t)\Delta_\alpha(t) , \quad \Delta_\mu(t) = -\frac{\partial}{\partial f_\mu}\mathcal{L}|_{f_\mu(t)}, \tag{2}$$

where we define base cases $G_{\mu\alpha}^{L+1}(t, s) = 1$, $\Phi_{\mu\alpha}^0(t, s) = K_{\mu\alpha}^x = \frac{1}{D}\boldsymbol{x}_\mu \cdot \boldsymbol{x}_\alpha$. The above expressions demonstrate that knowledge of the temporal trajectory of the NTK on the $t = s$ diagonal gives the temporal trajectory of the network predictions $f_\mu(t)$. Following prior works on infinite-width networks [21, 22, 45, 18], we study the mean field limit $N, \gamma \to \infty$, $\gamma_0 = \frac{\gamma}{\sqrt{N}} = \mathcal{O}_N(1)$. The $\gamma_0 = 0$ limit recovers the static NTK limit [6], while $\gamma_0 > 0$ allows feature learning.

3 Self-consistent DMFT

Next, we derive our self-consistent DMFT in a limit where $t, P = \mathcal{O}_N(1)$. Our goal is to build a description of training dynamics purely based on representations, and independent of weights. Studying feature learning at infinite-width enjoys several analytical properties:

- The kernel order parameters Φ^ℓ, G^ℓ concentrate over random initializations but are dynamical, allowing flexible adaptation of features to the task structure.

- In each layer ℓ, each neuron's preactivation h_i^ℓ and pregradient z_i^ℓ become i.i.d. draws from a distribution characterized by a set of order parameters $\{\Phi^\ell, G^\ell, A^\ell, B^\ell\}$.
- The kernels are defined as self-consistent averages (denoted by $\langle\rangle$) over this distribution of neurons in each layer $\Phi_{\mu\alpha}^\ell(t,s) = \langle\phi(h_\mu^\ell(t))\phi(h_\alpha^\ell(s))\rangle$ and $G_{\mu\alpha}^\ell(t,s) = \langle g_\mu^\ell(t)g_\alpha^\ell(s)\rangle$.

The next section derives these facts from a path-integral formulation of gradient flow dynamics.

3.1 Path Integral Construction

Gradient flow after a random initialization of weights defines a high dimensional stochastic process over initalizations for variables $\{h, g\}$. Therefore, we will utilize DMFT formalism to obtain a reduced description of network activity during training. Generally, we separate the contribution on each forward/backward pass between the initial condition and gradient updates to weight matrix W^ℓ, defining new stochastic variables $\chi_\mu^{\ell+1}(t) = \frac{1}{\sqrt{N}}W^\ell(0)\phi(h_\mu^\ell(t))$, $\quad \xi_\mu^\ell(t) = \frac{1}{\sqrt{N}}W^\ell(0)^\top g_\mu^{\ell+1}(t)$. We let Z represent the moment generating functional (MGF) for these stochastic fields

$$Z[\{j^\ell, v^\ell\}] = \left\langle \exp\left(\sum_{\ell,\mu} \int_0^\infty dt \left[j_\mu^\ell(t) \cdot \chi_\mu^\ell(t) + v_\mu^\ell(t) \cdot \xi_\mu^\ell(t) \right] \right) \right\rangle_{\{W^0(0),...w^L(0)\}}, \quad (3)$$

Performing integration over possible paths for χ^ℓ, ξ^ℓ, we show that the MGF Z can be described by set of order-parameters $\{\Phi^\ell, \hat{\Phi}^\ell, G^\ell, \hat{G}^\ell, A^\ell, B^\ell\}$ [23]

$$Z[\{j^\ell, v^\ell\}] \propto \int \prod_{\ell\mu\alpha ts} d\Phi_{\mu\alpha}^\ell(t,s)d\hat{\Phi}_{\mu\alpha}^\ell(t,s)dG_{\mu\alpha}^\ell(t,s)d\hat{G}_{\mu\alpha}^\ell(t,s)dA_{\mu\alpha}^\ell(t,s)dB_{\mu\alpha}^\ell(t,s) \quad (4)$$

$$\times \exp\left(NS[\{\Phi, \hat{\Phi}, G, \hat{G}, A, B, j, v\}] \right),$$

$$S = \sum_{\ell\mu\alpha} \int_0^\infty dt \int_0^\infty ds \left[\Phi_{\mu\alpha}^\ell(t,s)\hat{\Phi}_{\mu\alpha}^\ell(t,s) + G_{\mu\alpha}^\ell(t,s)\hat{G}_{\mu\alpha}^\ell(t,s) - A_{\mu\alpha}^\ell(t,s)B_{\mu\alpha}^\ell(t,s) \right]$$

$$+ \ln \mathcal{Z}[\{\Phi, \hat{\Phi}, G, \hat{G}, A, B, j, v\}], \quad (5)$$

where S is the DMFT action and $\mathcal{Z}$ is a single-site MGF, which defines the distribution of fields $\{\chi^\ell, \xi^\ell\}$ over the neural population in each layer. The order parameters A and B are related to the correlations between feedforward and feedback signals in the network.

3.2 Deriving the DMFT Equations from the Path Integral Saddle Point

As $N \to \infty$, the moment-generating function Z is exponentially dominated by the saddle point of S. The equations that define this saddle point also define our DMFT. We thus identify the kernels that render S locally stationary ($\delta S = 0$). The most important equations are those which define $\{\Phi^\ell, G^\ell\}$

$$\frac{\delta S}{\delta\hat{\Phi}_{\mu\alpha}^\ell(t,s)} = \Phi_{\mu\alpha}^\ell(t,s) + \frac{1}{\mathcal{Z}}\frac{\delta\mathcal{Z}}{\delta\hat{\Phi}_{\mu\alpha}^\ell(t,s)} = \Phi_{\mu\alpha}^\ell(t,s) - \langle\phi(h_\mu^\ell(t))\phi(h_\alpha^\ell(s))\rangle = 0,$$

$$\frac{\delta S}{\delta\hat{G}_{\mu\alpha}^\ell(t,s)} = G_{\mu\alpha}^\ell(t,s) + \frac{1}{\mathcal{Z}}\frac{\delta\mathcal{Z}}{\delta\hat{G}_{\mu\alpha}^\ell(t,s)} = G_{\mu\alpha}^\ell(t,s) - \langle g_\mu^\ell(t)g_\alpha^\ell(s)\rangle = 0, \quad (6)$$

where $\langle\rangle$ denotes an average over the stochastic process induced by $\mathcal{Z}$, which is defined below

$$\{u_\mu^\ell(t)\}_{\mu\in[P],t\in\mathbb{R}_+} \sim \mathcal{GP}(0, \Phi^{\ell-1}), \quad \{r_\mu^\ell(t)\}_{\mu\in[P],t\in\mathbb{R}_+} \sim \mathcal{GP}(0, G^{\ell+1}),$$

$$h_\mu^\ell(t) = u_\mu^\ell(t) + \gamma_0 \int_0^t ds \sum_{\alpha=1}^P \left[A_{\mu\alpha}^{\ell-1}(t,s) + \Delta_\alpha(s)\Phi_{\mu\alpha}^{\ell-1}(t,s) \right] z_\alpha^\ell(s)\dot{\phi}(h_\alpha^\ell(s)),$$

$$z_\mu^\ell(t) = r_\mu^\ell(t) + \gamma_0 \int_0^t ds \sum_{\alpha=1}^P \left[B_{\mu\alpha}^\ell(t,s) + \Delta_\alpha(s)G_{\mu\alpha}^{\ell+1}(t,s) \right] \phi(h_\alpha^\ell(s)), \quad (7)$$

where we define base cases $\Phi_{\mu\alpha}^0(t,s) = K_{\mu\alpha}^x$ and $G_{\mu\alpha}^{L+1}(t,s) = 1$, $A^0 = B^L = 0$. We see that the fields $\{h^\ell, z^\ell\}$, which represent the single site preactivations and pre-gradients, are implicit

functionals of the mean-zero Gaussian processes $\{u^\ell, r^\ell\}$ which have covariances $\langle u_\mu^\ell(t) u_\alpha^\ell(s) \rangle = \Phi_{\mu\alpha}^{\ell-1}(t,s)$ and $\langle r_\mu^\ell(t) r_\alpha^\ell(s) \rangle = G_{\mu\alpha}^{\ell+1}(t,s)$. The other saddle point equations give response functions $A_{\mu\alpha}^\ell(t,s) = \gamma_0^{-1} \left\langle \frac{\delta \phi(h_\mu^\ell(t))}{\delta r_\alpha^\ell(s)} \right\rangle, B_{\mu\alpha}^\ell(t,s) = \gamma_0^{-1} \left\langle \frac{\delta g_\mu^{\ell+1}(t)}{\delta u_\alpha^{\ell+1}(s)} \right\rangle$ which arise due to coupling between the feedforward and feedback signals. We note that, in the lazy limit $\gamma_0 \to 0$, the fields approach Gaussian processes $h^\ell \to u^\ell$, $z^\ell \to r^\ell$.

4   Solving the Self-Consistent DMFT

(a) Lazy vs Rich Loss Dynamics   (b) Initial Preactivation Density   (c) Final Preactivation Density

(d) Final Φ^ℓ Kernels $\gamma_0 = 1$ (e) Φ^ℓ Dynamics $\gamma_0 = 1.0$ (f) Φ^ℓ Convergence to DMFT

(g) Final G^ℓ kernels $\gamma_0 = 1.0$ (h) G^ℓ Dynamics $\gamma_0 = 1.0$ (i) G^ℓ Convergence to DMFT
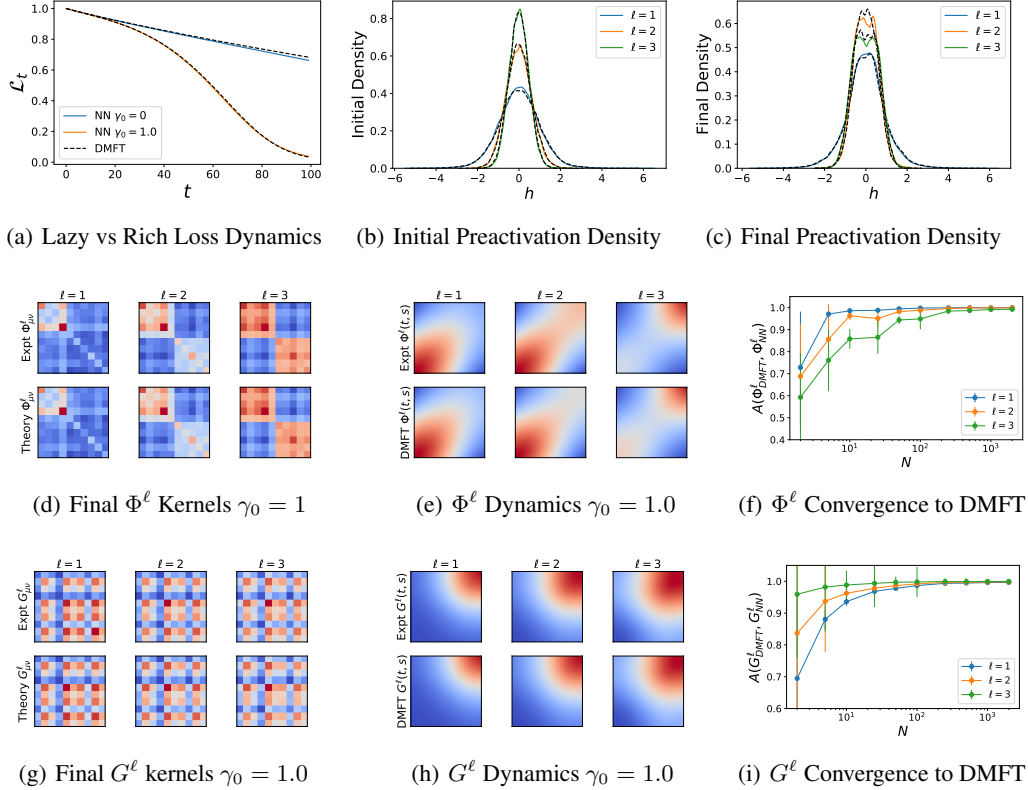
Figure 1: Neural network feature learning dynamics is captured by self-consistent dynamical mean field theory (DMFT). (a) Training loss curves on a subsample of $P = 10$ CIFAR-10 training points in a depth 4 ($L = 3$, $N = 2500$) tanh network ($\phi(h) = \tanh(h)$) trained with MSE. Increasing γ_0 accelerates training. (b)-(c) The distribution of preactivations at the beginning and end of training matches predictions of the DMFT. (d) The final Φ^ℓ (at $t = 100$) kernel order parameters match the finite width network. (e) The temporal dynamics of the sample-traced kernels $\sum_\mu \Phi_{\mu\mu}^\ell(t,s)$ matches experiment and reveals rich dynamics across layers. (f) The alignment $A(\mathbf{\Phi}_{DMFT}^\ell, \mathbf{\Phi}_{NN}^\ell)$, defined as cosine similarity, of the kernel $\Phi_{\mu\alpha}^\ell(t,s)$ predicted by theory (DMFT) and width N networks for different N but fixed $\gamma_0 = \gamma/\sqrt{N}$. Errorbars show standard deviation computed over 10 repeats. Around $N \sim 500$ DMFT begins to show near perfect agreement with the NN. (g)-(i) The same plots but for the gradient kernel $\mathbf{G}^\ell$. Whereas finite width effects for $\mathbf{\Phi}^\ell$ are larger at later layers ℓ since variance accumulates on the forward pass, fluctuations in $\mathbf{G}^\ell$ are large in early layers.

The saddle point equations obtained from the field theory discussed in the previous section must be solved self-consistently. By this we mean that, given knowledge of the kernels, we can characterize the distribution of $\{h^\ell, z^\ell\}$, and given the distribution of $\{h^\ell, z^\ell\}$, we can compute the kernels [46, 41]. We use a numerical procedure based on this idea to efficiently solve for the kernels with an alternating Monte-Carlo strategy. The output of the algorithm are the dynamical kernels $\Phi_{\mu\alpha}^\ell(t,s), G_{\mu\alpha}^\ell(t,s), A_{\mu\alpha}^\ell(t,s), B_{\mu\alpha}^\ell(t,s)$, from which any network observable can be computed. We

provide an example of the solution to the saddle point equations compared to training a finite NN in Figure 1. We plot Φ^ℓ, G^ℓ at the end of training and the sample-trace of these kernels through time. We compare kernels of finite width N network to the DMFT predicted kernels using a cosine-similarity alignment metric $A(\mathbf{\Phi}^{DMFT}, \mathbf{\Phi}^{NN}) = \frac{\text{Tr } \mathbf{\Phi}^{DMFT} \mathbf{\Phi}^{NN}}{|\mathbf{\Phi}^{DMFT}||\mathbf{\Phi}^{NN}|}$, with agreement at large N.

We can also compare the exact DMFT equations to approximation schemes employed in prior works on wide networks. Specifically, we compare static NTK (NTK), perturbative (Pert.) (leading corrections to feature evolution of size γ_0^2) [47] and gradient independence (Gr. Indep.) (backward pass weights approximated as independent of forward pass) [48]. In Figure 2, we show that only DMFT is accurate over a wide range of feature learning strengths γ_0.
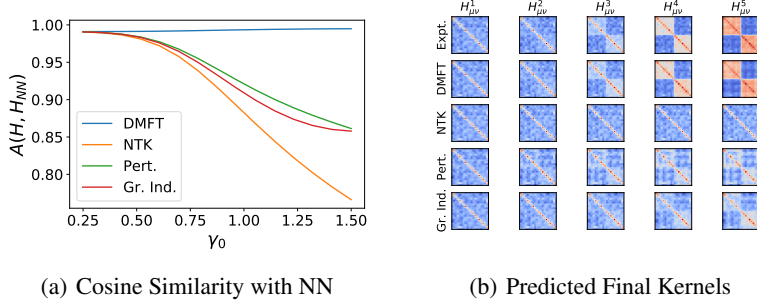

(a) Cosine Similarity with NN (b) Predicted Final Kernels

Figure 2: DMFT is accurate for wide range of γ_0, while other approximations including perturbation theory and gradient independence break down for large γ_0.

5   Broader Impacts

We provided a unifying DMFT derivation of feature dynamics in infinite networks trained with gradient based optimization. Our theory interpolates between lazy infinite-width behavior of a static NTK in $\gamma_0 \to 0$ and rich feature learning. At $\gamma_0 = 1$, our DMFT construction agrees with the stochastic process derived previously with the Tensor Programs framework [22]. Our saddle point equations give self-consistency conditions which relate the stochastic fields to the kernels. These equations are exactly solveable in deep linear networks and can be efficiently solved with a numerical method in the nonlinear case. Comparisons with other approximation schemes show that DMFT can be accurate at a much wider range of γ_0. We believe our framework could be a useful perspective for future theoretical analyses of feature learning and generalization in wide networks, including networks trained with alternative learning rules [49].

Though our DMFT is quite general in regards to the data and architecture, the technique is not entirely rigorous and relies on heuristic physics techniques. Our theory holds in the $T, P = \mathcal{O}_N(1)$ and may break down otherwise; other asymptotic regimes (such as $P/N, T/\log(N) = \mathcal{O}_N(1)$, etc) may exhibit phenomena relevant to deep learning practice [50, 51]. The computational requirements of our method, while smaller than the exponential time complexity for exact solution [22], are still significant for large PT. In Table 1, we compare the time taken for various theories to compute the feature kernels throughout T steps of gradient descent.

Requirements	Width-N NN	Static NTK	Perturbative	Full DMFT
Memory for Kernels	$\mathcal{O}(N^2)$	$\mathcal{O}(P^2)$	$\mathcal{O}(P^4 T)$	$\mathcal{O}(P^2 T^2)$
Time for Kernels	$\mathcal{O}(PN^2 T)$	$\mathcal{O}(P^2)$	$\mathcal{O}(P^4 T)$	$\mathcal{O}(P^3 T^3)$
Time for Final Outputs	$\mathcal{O}(PN^2 T)$	$\mathcal{O}(P^3)$	$\mathcal{O}(P^4)$	$\mathcal{O}(P^3 T^3)$

Table 1: Computational requirements to compute kernel dynamics and trained network predictions on P points in a depth N neural network on a grid of T time points trained with P data points for various theories. DMFT is faster and less memory intensive than a width N network only if $N \gg PT$. It is more computationally efficient to compute full DMFT kernels than leading order perturbation theory when $T \ll \sqrt{P}$.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes] As described in the abstract and introduction, we provide a dynamical field theory of deep networks based on kernel evolution.
   (b) Did you describe the limitations of your work? [Yes] We have an explicit limitations as the last paragraph of the paper in Section 5.
   (c) Did you discuss any potential negative societal impacts of your work? [N/A] This work is theoretical and is very unlikely to present negative social impacts.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] We describe that our theory holds for NN architectures in the infinite-width $N \to \infty$ limit.
   (b) Did you include complete proofs of all theoretical results? [Yes] All claims made in the main text are supported by derivations in the Appendix.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Code to reproduce experimental results is provided in the supplementary material.
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] We provide details of our experiments in 1
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] Mentioned 10 repeats in Figure 1 caption.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [N/A] This is a theory paper

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [N/A]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]

5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]