SPONTANEOUS SYMMETRY BREAKING IN DEEP NEURAL NETWORKS

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ABSTRACT

We propose a framework to understand the unprecedented performance and robustness of deep neural networks using field theory. Correlations between the weights within the same layer can be described by symmetries in that layer, and networks generalize better if such symmetries are broken to reduce the redundancies of the weights. Using a two parameter field theory, we find that the network can break such symmetries itself towards the end of training in a process commonly known in physics as spontaneous symmetry breaking. This corresponds to a network generalizing itself without any user input layers to break the symmetry, but by communication with adjacent layers. In the layer decoupling limit applicable to residual networks (He et al., 2015), we show that the remnant symmetries that survive the non-linear layers are spontaneously broken. The Lagrangian for the non-linear and weight layers together has striking similarities with the one in quantum field theory of a scalar. Using results from quantum field theory we show that our framework is able to explain many experimentally observed phenomena, such as training on random labels with zero error (Zhang et al., 2017), the information bottleneck and the phase transition out of it (Shwartz-Ziv & Tishby, 2017), shattered gradients (Balduzzi et al., 2017), and many more.

1 INTRODUCTION

Deep Neural Networks have been used in image recognition tasks with great success. The first of its kind, AlexNet (Krizhevsky et al., 2012), led to many other neural architectures have been proposed to achieve start-of-the-art results in image processing at the time. Some of the notable architectures include, VGG (Simonyan & Zisserman, 2015), Inception (Szegedy et al., 2015) and Residual networks (ResNet)(He et al., 2015).

Understanding the inner working of deep neural networks remains a difficult task until now. It has been discovered that the training progress ceases when it goes through an information bottleneck (Shwartz-Ziv & Tishby, 2017) until learning rate is decreased to a suitable amount then the network under goes a phase transition. Deep networks appear to be able to regularize themselves and able to train on randomly labeled data Zhang et al. (2017) with zero training error. The gradients in deep neural networks behaves as white noise over the layers Balduzzi et al. (2017). And many other unexplained phenomona. We have found a framework that can explain all the aforementioned results, among many others.

A recent work (Anonymous, 2018) showed that the ensemble behavior and binomial path lengths (Veit et al., 2016) of ResNets can be explained by just a Taylor series expansion to first order in the decoupling limit. They found that the series approximation generates a symmetry breaking layer that reduces the redundancy of weights, leading to a better generalization. Because the ResNet does not contain such symmetry breaking layers in the architecture. They suggest that ResNets are able to break the symmetry by the communication between the layers. Another recent work also employed the Taylor expansion to investigate ResNets (Jastrzebski et al., 2017).

We show that a remnant symmetry subgroup can survive a ReLU layer and the weights can be thought as scalar fields covariant to this remnant symmetry. The emergence of a scalar field is intriguing, perhaps troubling. A scalar field can admit negative Hessian eigenvalues at the loss minimum. Historically, this paradox is solved by promoting a scalar field theory to a quantum field theory incorporating Einstein's special relativity (Srednicki, 2007). But how does this apply

to neural networks? We now illustrate that a residual network behaves just like a quantum field theory. In the layer decoupling limit, the norm of the change in feature map representation through each layer has an upper bound, by definition of the layer decoupling. This is similar to relativity where the speed of any particle is bounded from above by the speed of light. In Residual networks, it has been shown that the network can be decomposed into a sum of subnetworks consisting of all possible paths between two layers Veit et al. (2016). In quantum mechanics, the propagation of particle between two points is the sum of all paths connecting those two points. So a residual network can be described by a quantum field theory and the use of a scalar field is justified. In fact, the presence of negative Hessian eigenvalues drives phase transitions in deep neural networks, and such eigenvalues also have also been observed (Chaudhari et al., 2017). We explain briefly the reason to go quantum in Appendix D.

Much of the literature on neural network design focuses on different neural architecture that breaks symmetry explicitly, rather than spontaneously. For instance, non-linear layers explicitly breaks the symmetry of affine transformations. There is little discussion on spontaneous symmetry breaking. In neural networks, the Goldstone theorem in field theory states that for every continuous symmetry that is spontaneously broken, there exists a weight with zero Hessian eigenvalue at the loss minimum. No such weights would appear if the symmetries are only explicitly broken, and not spontaneously. It turns out that many seemingly different experimental results can be explained by the presence of these zero eigenvalue weights. In this work, we exploit the layer decoupling limit applicable to ResNets to approximate the loss functions with a power series in symmetry invariant quantities and illustrate that spontaneous symmetry breaking of affine symmetries is the sufficient and necessary condition for a deep network to attain its unprecedented power.

The organization of this paper is as follows. The background on deep neural networks and field theory is given in Section 2. Section 3 shows that remnant symmetries can exist in a neural network and that the weights can be approximated by a scalar field. Experimental results that confirm our theory is given in Section 4. We summarize more evidence from other experiments in Appendix A. A review of field theory is given in Appendix B. An explicit example of spontaneous symmetry breaking is shown in Appendix C.

2 Background and Framework

In this section we introduce our frame work using a field theory based on Lagrangian mechanics.

2.1 Deep Neural Networks

A deep neural network consists of layers of neurons. Suppose that the first layer of neurons with weight matrix $\mathbf{W}_1'$ and bias $\mathbf{b}_1$ takes input $\mathbf{x}_1'$ and outputs $\mathbf{y}_1$

$$\mathbf{y}_1 = \mathbf{W}_1'\mathbf{x}_1' + \mathbf{b}_1 = \mathbf{W}_1\mathbf{x}_1,$$

where $\mathbf{x} = (\mathbf{x}', 1)$ and $\mathbf{W}_1 = (\mathbf{W}_1', \mathbf{b}_1)$, where $\mathbf{W}_1$ and $\mathbf{b}_1$ are real valued. Now suppose that R_1 denotes a nonlinear operator corresponding to a sigmoid or ReLU layer located after the weight layer, so that

$$\mathbf{y}_1 = R_1\mathbf{W}_1\mathbf{x}_1.$$

For a neural network with T repeating units, the output for layer t is

$$\begin{aligned} \mathbf{y}_t &= R_t\mathbf{W}_t\mathbf{y}_{t-1} \\ &= R_t\mathbf{W}_t R_{t-1}\mathbf{W}_{t-1}\ldots R_1\mathbf{W}_1\mathbf{x}_1 \\ &= \left(\prod_{n=0}^{t-1} R_{t-n}\mathbf{W}_{t-n}\right)\mathbf{x}_1. \end{aligned} \tag{1}$$

2.2 Symmetries in Neural Networks

We now show the necessary and sufficient conditions of preserving symmetry. We explicitly include symmetry transformations in Equation (1) and investigate the effects caused by a symmetry transformation of the input in subsequent layers. Suppose $Q_t \in G$ is a transformation matrix in some

Lie group G for all t. Note that the Q_t are not parameters to be estimated. We write $\mathbf{y}_t = \mathbf{y}_t(Q_t)$, where the dependence on Q_t is obtained from a transformation on the input, $\mathbf{x}_t(Q_t) = Q_t\mathbf{x}_t$, and the weights, $\mathbf{W}_t(Q_t)$

$$\mathbf{y}_t(Q_t) = R_t\mathbf{W}_t(Q_t)\mathbf{x}_t(Q_t).$$

If G is a symmetry group, then $\mathbf{y}_t$ is covariant with $\mathbf{x}_t$, such that $\mathbf{y}_t(Q_t) = Q_t\mathbf{y}_t$. This requires two conditions to be satisfied. First, $\mathbf{W}_t(Q_t) = Q_t\mathbf{W}_tQ_t^{-1}$, where $Q_t^{-1}Q_t = I$ and the existence of the inverse is trivial because G is a group and $Q_t \in G$. The second is the commutativity between R_t and Q_t, such that $R_tQ_t = Q_tR_t$. For example, if $g_t \in \text{Aff}(D)$, the group of affine transformations, R_t may not commute with g_t. However, commutativity is satisfied when the transformation corresponds to the 2D rotation of feature maps.

Including transformation matrices, the output at layer t is

$$\mathbf{y}_t(Q_t) = \left(\prod_{n=0}^{t-1} R_{t-n}Q_{t-n}\mathbf{W}_{t-n}Q_{t-n}^{-1}\right)Q_1\mathbf{x}_1.$$

2.3 The Loss Functional

Statistical learning requires the loss function to be minimized. It can be written in the form of a mutual information, training error, or the Kullback-Leibler divergence. In this section we approximate the loss function in the continuum limit of samples and layers. Then we define the loss functional to transition into Lagrangian mechanics and field theory. Let $\mathbf{z}_i = (\mathbf{X}_i, \mathbf{Y}_i) \in \mathcal{X}$ be the i-th input sample in data set $\mathcal{X}$, $(\mathbf{X}_i, \mathbf{Y}_i)$ are the features and the desired outputs, respectively, and $i \in \{1, \ldots, N\}$. The loss function is

$$L = \frac{1}{N}\sum_{i=1}^{N} L_i(\mathbf{X}_i, \mathbf{Y}_i, \mathbf{W}, \mathbf{Q}),$$

where $\mathbf{W} = (\mathbf{W}_1, \ldots, \mathbf{W}_T)$, and $\mathbf{Q} = (Q_1, \ldots, Q_T)$, $Q_t \in G$ where G is a Lie group, and T is the depth of the network. Taking the continuum limit,

$$L \simeq \int_{\mathcal{X}} p(\mathbf{X}, \mathbf{Y})L_{\mathbf{x}}(\mathbf{X}, \mathbf{Y}, \mathbf{W}, \mathbf{Q})d\mathbf{X}d\mathbf{Y},$$

where $p(\mathbf{X}, \mathbf{Y})$ is the joint distribution of $\mathbf{X}$ and $\mathbf{Y}$. Using the first fundamental theorem of calculus and taking the continuous layers (t) limit, we write

$$L_{\mathbf{x}} \simeq L_{\mathbf{x}}(t = 0) + \int_0^T \frac{dL_{\mathbf{x}}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q(t))}{dt}dt,$$

where $L_{\mathbf{x}}(t = 0)$ is the value of the loss before training. We let $L_{\mathbf{x},t} = dL_{\mathbf{x}}/dt$ be the loss rate per layer. The loss rate $L_{\mathbf{x},t}$ is bounded from below. Therefore

$$\min_{\mathbf{W}} L_{\mathbf{x}}(\mathbf{X}, \mathbf{Y}, \mathbf{W}, \mathbf{Q}) = L_{\mathbf{x}}(t = 0) + \int_0^T \min_{\mathbf{W}_t} L_{\mathbf{x},t}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q(t))dt.$$

Minimizing the loss rate guarantees the minimization of the total loss. We require $L_{\mathbf{x},t}$ to be invariant under symmetry transformations. That is, if $Q_1(t), Q_2(t) \in G$. Then

$$L_{\mathbf{x},t}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q_1(t)) = L_{\mathbf{x},t}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q_2(t)).$$

However if $Q_1(t)$ and $Q_2(t)$ do not belong in the same symmetry group, the above equality does not necessarily hold. Now we define the loss functional for a deep neural network

$$\mathcal{P}[\mathbf{W}, Q] = \int_{\mathcal{X}\times\{0,T\}} p(\mathbf{X}, \mathbf{Y})L_{\mathbf{x},t}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q(t))d\mathbf{X}d\mathbf{Y}dt.$$

2.4 Lagrangian mechanics and Field theory

Having defined the loss functional now, we can transition into Lagrangian dynamics to give a description of the feature map flow at each layer. Let the minimizer of the loss rate be

$$\mathbf{W}^*(\mathbf{X}, \mathbf{Y}, Q(t), t) = \arg\min_{\mathbf{W}} p(\mathbf{X}, \mathbf{Y})L_{\mathbf{x},t}(\mathbf{X}, \mathbf{Y}, \mathbf{W}(t), Q(t)).$$

From now on, we combine $\mathbf{z} = (\mathbf{X}, \mathbf{Y})$ as $\mathbf{Y}$ only appears in $\mathbf{W}^*$ in this formalism, each $\mathbf{Y}$ determines a trajectory for the feature map representation flow determined by Lagrangian mechanics. Now we define, for each i-th element of $\mathbf{W}(t)$,

$$v^i(\mathbf{z}, Q(t), t) = W^i(\mathbf{z}, Q(t)) - W^{*i}(\mathbf{z}, Q(t), t),$$

and we set the weights with a non-linear operator $R(t)$ together such that, $w^i(\mathbf{z}, Q(t), t) = R(t)v^i(\mathbf{z}, Q(t), t)$. We now define the Lagrangian density,

$$\mathcal{L} = \mathcal{L}(\mathbf{z}, \mathbf{w}, \partial_t \mathbf{w}, \partial_{\mathbf{z}} \mathbf{w}, Q(t))$$

and $\mathcal{L} = \mathcal{T} - \mathcal{V}$, where $\mathcal{T}$ is the kinetic energy and $\mathcal{V}$ is the potential energy. We define the potential energy to be

$$\mathcal{V} = p(\mathbf{z}) L_{\mathbf{x},t}(\mathbf{z}, \mathbf{W}(t), Q(t)),$$

The probability density $p(\mathbf{z})$ and the loss rate $L_{\mathbf{x},t}$ are invariant under symmetry transformations. Then $\mathcal{V}$ is an invariant as well.

Definition: Orthogonal Group The orthogonal group O(D) is the group of all $D \times D$ matrices such that $O^T O = I$.

We now set up the conditions to obtain a series expansion of $\mathcal{V}$ around the minimum $w^i(Q_t) = 0$. First, since $\mathcal{V}$ is an invariant. Each term in the series expansion must be an invariant such that $f(w_i(Q_t), w^i(Q_t)) = f(w_i, w^i)$ for all $Q_t \in G$. Suppose $G = O(D)$, the orthogonal group and that $\mathbf{w}^T(Q_t) = \mathbf{w}^T Q^T$ and $\mathbf{w}(Q_t) = Q_t \mathbf{w}$. So $w_i w^i$ is an invariant. Then $f = w_i w^i$ is invariant for all Q_t where the Einstein summation convention was used

$$w_i w^i = \sum_{i=1}^{D} w_i w^i = \mathbf{w}^T \mathbf{w},$$

Now we perform a Taylor series expansion about the minimum $w^i = 0$ of the potential,

$$\mathcal{V} = C + w_i H^i_j w^j + w_i w_j \Lambda^{ij}_{mn} w^m w^n + O((w_i w^i)^6),$$

where $H^i_j = \partial_{w^i} \partial_{w^j} \mathcal{V}$ is the Hessian matrix, and similarly for Λ^{ij}_{mn}. Because $\mathcal{V}$ is an even function in w^i around the minimum, we must have

$$w_i H^i_j w^j = \sum_{i=1}^{D} w_i H^i_i w^i.$$

The O(D) symmetry enforces that all weight Hessian eigenvalues to be $H^i_i = m^2/2$ for some constant m^2. This can be seen in the O(2) case, with constants a, b, $a \neq b$, $Q \in$ O(2) such that $w_1(Q) = w_2$ and $w_2(Q) = w_1$,

$$a w_1(Q)^2 + b w_2(Q)^2 = a w_2^2 + b w_1^2,$$

this does not equal $a w_1^2 + b w_2^2$, so the O(2) symmetry implies $a = b$. This can be generalized to the O(D) case. For the quartic term, the requirement that $\mathcal{V}$ be even around the minimum gives

$$w_i w_j \Lambda^{ij}_{mn} w^m w^n = \sum_{i,j=1}^{D} \Lambda^{ij}_{ij} w_j w^j w_i w^i.$$

Similarly the O(D) symmetry implies $\Lambda^{ii}_{ii} = \lambda/4$ for some constant λ and zero for any other elements, the potential is

$$\mathcal{V} = \frac{m^2}{2} w_i w^i + \frac{\lambda}{4} (w_i w^i)^2,$$

where the numerical factors were added for convention. The power series is a good approximation in the decoupling limit which may be applicable for Residual Networks.[1] For the kinetic term $\mathcal{T}$, we expand in power series of the derivatives,

$$\mathcal{T} = \frac{1}{2} \frac{\partial w_i}{\partial t} \frac{\partial w^i}{\partial t} - \frac{1}{2} \frac{1}{c^2} \frac{\partial w_i}{\partial \mathbf{z}} \frac{\partial w^i}{\partial \mathbf{z}} + O((\partial_t w)^4, (\partial_{\mathbf{z}} w)^4),$$

[1] The output of a residual unit is $\mathbf{y}_t = \mathbf{x}_t + \mathbf{F}_t(\mathbf{x}_t, \mathbf{W}_{1t}, \mathbf{W}_{2t})$, with $\mathbf{F}_t \ll \mathbf{x}_t$. Omitting non-linear layers, $\mathbf{F}_t(\mathbf{x}_t, \mathbf{W}_{1t}, \mathbf{W}_{2t}) = \mathbf{W}_{t2} \mathbf{W}_{t1} \mathbf{x}_t$. This means the pair of weights in adjacent layers is small also.

where the coefficient for $(\partial_t w)^2$ is fixed by the Hamiltonian kinetic energy $\frac{1}{2}(\partial_t w)^2$. Higher order terms in $(\partial_t w)^2$ are negligible in the decoupling limit. If the model is robust, then higher order terms in $(\partial_{\mathbf{z}} w)^2$ can be neglected as well. [2] The Lagrangian density is [3]

$$\mathcal{L} = \frac{1}{2}(\partial_t w)^2 - \frac{1}{2}(\partial_{\mathbf{z}} w)^2 - \frac{m^2}{2} w^2 - \frac{\lambda}{4}(w^2)^2,$$

where we have set $w^2 = w_i w^i$ and absorbed c into $\mathbf{x}$ without loss of generality. This is precisely the Lagrangian for a scalar field in field theory. Standard results for a scalar field theory can be found in Appendix B. To account for the effect of the learning rate, we employ the results from thermal field theory (Kapusta & Gale, 2006) and we identify the temperature with the learning rate η. So that now $m^2 = -\mu^2 + \frac{1}{4}\lambda\eta^2$, with $\mu^2 > 0$.

2.5 Spontaneous Symmetry Breaking

Spontaneous symmetry breaking describes a phase transition of a deep neural network. Consider the following scalar field potential invariant under O(D') transformations,

$$\mathcal{V}(w^i, \eta) = \frac{m^2(\eta)}{2} w_i w^i + \frac{\lambda}{4}(w_i w^i)^2,$$

where $m^2(\eta) = -\mu^2 + \frac{1}{4}\lambda\eta^2$, $\mu^2 > 0$ and learning rate η. There exists a value of $\eta = \eta_c$ such that $m^2 = 0$. In the first phase, $\eta > \eta_c$, the loss minimum is at $w^*_{0i} = 0$, where

$$w^*_{0i}(\eta) = \arg\min_{w^i} \mathcal{V}(w^i, \eta).$$

When the learning rate η drops sufficiently low, the symmetry is spontaneously broken and the phase transition begins. The loss minimum bifurcates at $\eta = \eta_c$ into

$$w^*_i(\eta < \eta_c) = \pm\sqrt{\frac{-m^2(\eta)}{\lambda}}.$$

This occurs when the Hessian eigenvalue becomes negative, $m^2(\eta) < 0$, when $\eta < \eta_c$.

This phenomenon has a profound implication. It is responsible for phase transition in neural networks and generates long range correlation between the input and output. Details from field theory can be found in Appendix C. Figure 1 depicts the shape of the loss function during spontaneous symmetry breaking with a weight w. At $\eta > \eta_c$, the loss function has a loss minima at point A. When the learning rate decreases, such that $\eta < \eta_c$, the critical point at A becomes unstable and new minima with equal loss are generated. The weight must go through B to get to the new minimum C. If the learning rate is too small, the weight will be stuck near A. This explains why a cyclical learning rate can outperform a monotonic decreasing learning rate (Smith & Topin, 2017).

Because the broken symmetric is still respected by the loss function, any new minima generated from spontaneous symmetry breaking must have the same loss. If there is an unbroken continuous symmetry remaining, there would be a connected loss surface corresponding to the new minima respecting the unbroken symmetry. Spontaneous symmetry breaking splits the weights into two sets, $w \to (\pi, \sigma)$. The direction along this degenerate minina in weight space corresponds to π. And the direction in weight space orthogonal to π is σ. This has been shown experimentally by Goodfellow et al. (2014) in Figure 19.

3 Symmetries in Neural Networks

In this section we show that spontaneous symmetry breaking occurs in neural networks. First, we show that learning by deep neural networks can be considered solely as breaking the symmetries in

[2] The kinetic term $\mathcal{T}$ is not invariant under transformation $Q(t)$. To obtain invariance $\partial_t w^i$ is to be replaced by the covariant derivative $D_t w^i$ so that $(D_t w^i)^2$ is invariant under $Q(t)$, (Peskin & Schroeder, 1995). $D_t w^i(\mathbf{z}, t, Q(t)) = \partial_t w^i(\mathbf{z}, t, Q(t)) + \alpha B(\mathbf{z}, t, Q(t))^i_j w^j(\mathbf{z}, t, Q(t))$, with $\mathbf{B}(\mathbf{z}, t, Q_t) = Q(t)B(\mathbf{z}, t)Q(t)^{-1}$. The new fields $\mathbf{B}$ introduced for invariance is not responsible for spontaneous symmetry breaking, the focus of this paper. So we will not consider them further.

[3] Formally, the $\partial_{\mathbf{z}} w$ term should be part of the potential $\mathcal{V}$, as $\mathcal{T}$ contains only $\partial_t w$ terms. However we adhere to the field theory literature and put the $\partial_{\mathbf{z}} w$ term in $\mathcal{T}$ with a minus sign, owning to $\mathcal{L} = \mathcal{T} - \mathcal{V}$.

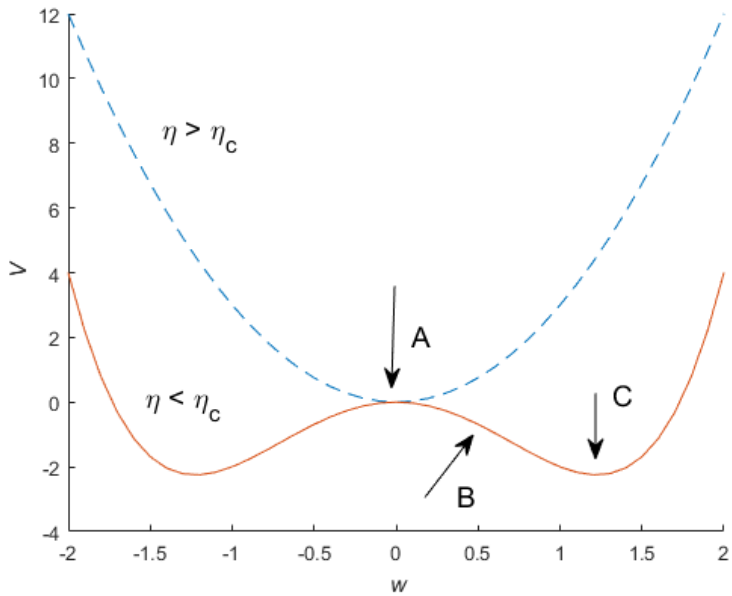

Figure 1: The characteristics of the loss function with spontaneous symmetry breaking. The dashed line corresponds to the symmetric phase, while the solid line corresponds to the broken phase.

the weights. Then we show that some non-linear layers can preserve symmetries across the non-linear layers. Then we show that weight pairs in adjacent layers, but not within the same layer, is approximately an invariant under the remnant symmetry leftover by the non-linearities. We assume that the weights are scalar fields invariant under the orthogonal O(D') group for some D' and find that experimental results show that deep neural networks undergo spontaneous symmetry breaking.

Theorem: Deep feedforward networks learn by breaking symmetries *Proof*: Let A_i be an operator representing any sequence of layers, and let a network formed by applying A_i repeatedly such that $x_{out} = (\prod_{i=1}^{M} A_i)x_{in}$. Suppose that $A_i \in$ Aff(D), the symmetry group of all affine transformations. We have $L = \prod_{i=1}^{D} A_i$, where $L \in$ Aff(D). Then $x_{out} = Lx_{in}$ for some $L \in$ Aff(D) and x_{out} can be computed by a single affine transformation L. When A_i contains a non-linearity for some i, this symmetry is explicitly broken by the nonlinearity and the layers learn a more generalized representation of the input. □

Now we show that ReLU preserves some continuous symmetries.

Theorem: ReLU reduces the symmetry of an Aff(D) invariant to some subgroup Aff(D'), where $D' < D$. *Proof*: Suppose R denotes the ReLU operator with output $\mathbf{y}_t$ and $Q_t \in$ Aff(D) acts on the input $\mathbf{x}_t$, where $R(\mathbf{x}) = \max(0, \mathbf{x})$. Let $\mathbf{x}^T\mathbf{x}$ be an invariant under $Q \in$ Aff(D) and let $\mathbf{x}^T = (\gamma, \nu)$, $\nu < 0$ and $\gamma > 0$. Let $\mathbf{a} = R\mathbf{x} = (\gamma, 0)$. Then $\mathbf{a}^T\mathbf{a} = \mathbf{x}^T R R\mathbf{x} = \gamma^T\gamma$. Then $\mathbf{a}^T\mathbf{a}$ is an invariant under Aff(D') where $D' = \dim\gamma$. Note that γ^i can be transformed into a negative value as it has passed the ReLU already. □

Corollary If there exist some $Q \in$ G that commutes with a nonlinear operator R, such that $QR = RQ$, then R preserves the symmetry G.

Definition: Remnant Symmetry If $Q_t \in G$ commutes with a non-linear operator R_t for all Q_t, then G is a remnant symmetry at layer t.

For the loss function $L_i(\mathbf{X}_i, \mathbf{Y}_i, \mathbf{W}, \mathbf{Q})$ to be invariant, we need the predicted output $\mathbf{y}_T$ to be covariant with $\mathbf{x}_i$. Similarly for an invariant loss rate $L_{\mathbf{x},t}$ we require $\mathbf{y}_t$ to be covariant with $\mathbf{x}_t$.

The following theorem shows that a pair of weights in adjacent layers can be considered an invariant for power series expansion.

Theorem: Neural network weights in adjacent layers form an approximate invariant Suppose a neural network consists of affine layers followed by a continuous non-linearity, R_t, and that the weights at layer t, $\mathbf{W}_t$ transform as $Q_t\mathbf{W}_tQ_t^{-1}$, and that $Q_t \in H$ is a remnant symmetry such that $Q_tR_t = R_tQ_t$. Then $\mathbf{W}_t\mathbf{W}_{t-1}$ can be considered as an invariant for the loss rate.

Proof: Consider $\mathbf{x}(Q_t) = Q_t\mathbf{x}_t$, then

$$\begin{aligned}\mathbf{y}_t(Q_t) &= R_t\mathbf{W}_t(Q_t)\mathbf{x}_t(Q_t)\\ &= R_tQ_t\mathbf{W}_tQ_t^{-1}Q_t\mathbf{x}_t\\ &= R_tQ_t\mathbf{W}_t\mathbf{x}_t\\ &= Q_tR_t\mathbf{W}_t\mathbf{x}_t,\end{aligned}$$

where in the last line $Q_tR_t = R_tQ_t$ was used, so $\mathbf{y}_t(Q_t) = Q_t\mathbf{y}_t$ is covariant with $\mathbf{x}_t$. Now, $\mathbf{x}_t = R_{t-1}\mathbf{W}_{t-1}\mathbf{x}_{t-1}$, so that

$$\mathbf{y}_t(Q_t) = Q_tR_t\mathbf{W}_tR_{t-1}\mathbf{W}_{t-1}\mathbf{x}_{t-1}.$$

The pair $(R_t\mathbf{W}_t)(R_{t-1}\mathbf{W}_{t-1})$ can be considered an invariant under the ramnant symmetry at layer t. Recall that $\mathbf{w}_t = R_t(\mathbf{W}_t - \mathbf{W}_t^*)$. Therefore $\mathbf{w}_t\mathbf{w}_{t-1}$ is an invariant. □

In the continuous layer limit, $\mathbf{w}_t\mathbf{w}_{t-1}$ tends to $\mathbf{w}(t)^T\mathbf{w}(t)$ such that $\mathbf{w}(t)$ is the first layer and $\mathbf{w}(t)^T$ corresponds to the one after. Therefore $\mathbf{w}(t)$ can be considered as a scalar field under the remnant symmetry. The remnant symmetry is not exact in general. For sigmoid functions it is only an approximation. The crucial feature for the remnant symmetry is that it is continuous so that strong correlation between inputs and outputs can be generated from spontaneous symmetry breaking. We will state the Goldstone Theorem from field theory without proof.

Theorem (Goldstone) For every spontaneously broken continuous symmetry, there exist a weight π with zero eigenvalue in the Hessian $m_\pi^2 = 0$.

In any case, we will adhere to the case where the remnant symmetry is an othogonal group $\mathrm{O}(D')$. Note that $\mathbf{W}$ is a $D \times D$ matrix and $D' < D$. We choose a subset $\mathbf{\Gamma} \in \mathbb{R}^{D'}$ of $\mathbf{W}$ such that $\mathbf{\Gamma}^T\mathbf{\Gamma}$ is invariant under $\mathrm{O}(D')$. Now that we have an invariant, we can write down the Lagrangian for a deep feedforward network for the weights responsible for spontaneous symmetry breaking.

The Lagrangian for deep feedforward networks in the decoupling limit Let $\gamma^i = R(\Gamma^i - \Gamma^{*i})$, using Equation (2)

$$\mathcal{L} = \frac{1}{2}(\partial_t\gamma^i)^2 - \frac{1}{2}(\partial_{\mathbf{z}}\gamma^i)^2 - \frac{m^2(\eta)}{2}\gamma^i\gamma_i - \frac{\lambda}{4}(\gamma^i\gamma_i)^2. \tag{2}$$

Now we can use standard field theory results and apply it to deep neural networks. A review for field theory is given in Appendix B. The formalism for spontaneous symmetry breaking is given in Appendix C.

4 Main Results

According to the Goldstone theorem, spontaneous symmetry breaking splits the set of weight deviations γ into two sets (σ, π) with different behaviors. Weights π with zero eigenvalues and a spectrum dominated by small frequencies $\mathbf{k}$ in its correlation function.[4] The other weights σ, have Hessian eigenvalues μ^2 as the weights before the symmetry is broken. In Appendix C, a standard calculation in field theory shows that the correlation functions of the weights have the form

$$P_{\sigma,\pi}(t, \mathbf{k}) = \frac{i}{2\omega_0}\exp\Big(-i\omega_0 t\Big), \tag{3}$$

[4]Please note that this does not have the same as the correlation in statistics. In statistical mechanics this is interpreted as a measure of the similarity between two functions at two different points. Please see Appendix B.

where $\omega_0 = \sqrt{|\mathbf{k}|^2 + m_{\sigma,\pi}^2}$, $m_\sigma^2 = -\mu_\sigma^2 + \frac{1}{4}\lambda\eta^2$ and $m_\pi^2 = \frac{1}{4}\lambda\eta^2$. The correlation function of π approaches infinity as $\mathbf{k} \to 0$, as $m_\pi^2 \to 0$. This corresponds to large correlation over all sample space *and* layers t.

Spontaneous symmetry breaking and the information bottleneck The neural network undergoes a phase transition out of the information bottleneck via spontaneous symmetry breaking described in Section 2.5. Before the phase transition, the weights γ have positive Hessian eigenvalues m^2. After the phase transition, weights π with zero Hessian eigenvalues are generated by spontaneous symmetry breaking. The correlation function for the π weights is concentrated around small values of $|\mathbf{k}|$, see Equation (3), with $\omega_0 = |\mathbf{k}|$ for any t. This corresponds to a highly correlated feature map representations across the sample (input) space and layers. Because the loss is minimized, the feature maps across the network is highly correlated with the desired output. And a large correlation across the sample space means that the feature map representations are independent of the input. This is precisely the behaviors observed by Shwartz-Ziv & Tishby (2017).

Gradient variance explosion It has been shown that the variance in weight gradients in the same layer grow by an order of magnitude during the end of training (Shwartz-Ziv & Tishby, 2017). We also connect this to spontaneous symmetry breaking. As two sets of weights, (σ, π) are generated with different distributions. Considering them as the same object would result in a larger variance.

Robustness of deep neural networks We find that neural networks are resilient to overfitting. Recall that the fluctuation in the weights can arise from sampling noise. Then $(\partial_{\mathbf{z}} w^i)^2$ can be a measure of model robustness. A small value denotes the weights' resistance to sampling noise. If the network were to overfit, the weights would be very sensitive to sampling error. After spontaneous symmetry breaking, weights with zero eigenvalues obey the Klein-Gordon equation with $m_\pi^2 = 0$,

$$(\partial_{\mathbf{z}}\pi)^2 = (\partial_{\mathbf{z}}\pi^*)(\partial_{\mathbf{z}}\pi) = |\mathbf{k}|^2, \quad \pi = \exp(i\omega t - i\mathbf{k}\cdot\mathbf{z}).$$

The singularity in the correlation function suggests $|\mathbf{k}|^2 \simeq 0$. The zero eigenvalue weights provide robustness to the model. Zhang et al. (2017) referred to this phenomenon as implicit regularization. This is independent of the data distribution. Therefore the network can learn data with random labels, also observed by Zhang et al. (2017).

The same argument hold to explain a recent result that in the presence of class imbalance, oversampling in convolution neural networks do not necessarily lead to overfitting (Buda et al., 2017).

5 Concluding Remarks

In this work we solved one of the most puzzling mysteries of deep learning by showing that deep neural networks undergo spontaneous symmetry breaking. This is a first attempt to describe a neural network with a scalar quantum field theory. We have shed light on many unexplained phenomenon observed in experiments, summarized in Appendix A.

One may wonder why our theoretical model works so well explaining the experimental results with just two parameters. It is all due to the decoupling limit such that a power series in the loss function is a good approximation to the network. In our case, the two expansion coefficients are the lowest number of possible parameters that is able to describe the phase transition observed near the end of training, where the performance of the deep network improves drastically. It is no concidence that our model can explain the empirical observations after the phase transition. In fact, our model can describe, at least qualitatively, the behaviors of phase transition in networks that the decoupling limit may not apply to. This suggests that the interations of nearby layers are responsible for the phase transition.

A Validation of Proposed Framework for Neural Networks in the Literature

In this section we summarize other experimental findings that can be explained by the proposed field theory and the perspective of symmetry breaking. Here $Q \in G$ acts on the the input and hidden variables $\mathbf{x}, \mathbf{h}$, as $Q\mathbf{x}, Q\mathbf{h}$.

- The shape of the loss function after spontaneous symmetry breaking has the same shape observed by Goodfellow et al. (2014) towards the end of training.
- A cyclical learning rate (Smith & Topin, 2017) helps to get to the new minimum faster, see Section 2.5.
- Results from Shwartz-Ziv & Tishby (2017) are due to spontaneous symmetry breaking, see Section 4.
- Identity mapping outperforms other skip connections (He et al., 2016) is a result of the residual unit's output being small. Then the residual units can be decoupled leading to a small λ and so it is easier for spontaneous symmetry breaking to occur, from $m^2 = -\mu^2 + \frac{1}{4}\lambda\eta^2$.
- Skip connection across residual units breaks additional symmetry. Suppose now an identity skip connection connects $\mathbf{x}_1$ and the output of $\mathbf{F}_2$. Now perform a symmetry transformation on $\mathbf{x}_1$ and $\mathbf{x}_2$, Q_1 and $Q_2 \in G$, respectively. Then the output after two residual untis is $Q\mathbf{x_3} = Q_1\mathbf{x_1} + Q_2\mathbf{x}_2 + Q_2\mathbf{F}_2$. Neither $Q = Q_1$ nor $Q = Q_2$ can satisfies the covariance under G. This is observed by Orhan & Pitkow (2017).
- The shattered gradient problem (Balduzzi et al., 2017). It is observed that the gradient in deep (non-residual) networks is very close to white noise. This is reflected in the exponential in Equation (6). This effect on ResNet is reduced because of the decoupling limit $\lambda \to 0$. This leads to the weight eigenvalues m^2 being larger in non-residual networks owing to $m^2 = -\mu^2 + \frac{1}{4}\lambda\eta^2$. And so a higher oscillation frequency in the correlation function.
- In recurrent neural networks, multiplicative gating (Yuhuai et al., 2016) combines the input $\mathbf{x}$ and the hidden state $\mathbf{h}$ by an element-wise product. Their method outperforms the method with an addition $\mathbf{x}+\mathbf{h}$ because the multiplication gating breaks the covariance of the output. A transformation $Q\mathbf{x} * Q\mathbf{h} \neq Q(\mathbf{x} * \mathbf{h})$, whereas for addition the output remains covariant $Q\mathbf{x} + Q\mathbf{h} = Q(\mathbf{x} + \mathbf{h})$.

B Review of Field Theory

In this section we state the relevant results in field theory without proof. We use Lagrangian mechanics for fields $w(\mathbf{x}, t)$. Equations of motion for fields are the solution to the Euler-Lagrange equation, which is a result from the principle of least action. The action, S, is

$$S[w] = \int L(t, w, \partial_t w) dt,$$

where L is the Lagrangian. Define the Lagrangian density

$$L(t) = \int \mathcal{L}(\mathbf{z}, t, w, \partial_{\mathbf{z},t} w) d\mathbf{z}.$$

The action in term of the Lagrangian density is

$$S[w] = \int \mathcal{L}(\mathbf{z}, t, w, \partial_{\mathbf{z},t} w) d\mathbf{z} dt.$$

The Lagrangian can be written as a kinetic term $\mathcal{T}$, and a potential term $\mathcal{V}$ (loss function),

$$\mathcal{L} = \mathcal{T} - \mathcal{V}$$

For a real scalar field $w(\mathbf{x}, t)$,

$$\mathcal{T} = \frac{1}{2}\left(\frac{\partial w}{\partial t}\right)^2 - \frac{1}{2}\frac{1}{c^2}\left(\frac{\partial w}{\partial \mathbf{z}}\right)^2 = \frac{1}{2}(\partial_t w)^2 - \frac{1}{2}(\partial_{\mathbf{z}} w)^2$$

where we have set the constant $c^2 = 1$ without loss of generality. The potential for a scalar field that allows spontaneous symmetry breaking has the form

$$\mathcal{V} = \frac{m^2}{2} w^2 + \frac{\lambda}{4} w^4.$$

In the decoupling limit, $\lambda \to 0$, the equation of motion for w is the Klein-Gordon Equation

$$[(\partial_t)^2 - (\partial_{\mathbf{z}})^2 - m^2]w = 0.$$

In the limit of $m^2 \to 0$, the Klein-Gordon Equation reduces to the wave equation with solution

$$w(\mathbf{z}, t) = e^{i(\omega t - \mathbf{k}\cdot\mathbf{z})},$$

where $i = \sqrt{-1}$.

One can treat w as a random variable such that the probability distribution (a functional) of the scalar field $w(\mathbf{z}, t)$ is $p[w] = \exp(-S[w])/\mathcal{Z}$, where $\mathcal{Z}$ is some normalizing factor. The distribution peaks at the solution of the Klein-Gordon equation since it minimizes the action S. Now we can define the correlation function between $w(\mathbf{z}_1, t_1)$ and $w(\mathbf{z}_2, t_2)$,

$$\langle w(\mathbf{z}_1, t_1) w(\mathbf{z}_2, t_2)\rangle = \frac{1}{\mathcal{Z}} \int w(\mathbf{z}_1, t_1) w(\mathbf{z}_2, t_2) e^{-S[w]} \mathcal{D}w,$$

where $\int \mathcal{D}w$ denotes the integral over all paths from $(\mathbf{z}_1, t_1)$ to $(\mathbf{z}_2, t_2)$. In the decoupling limit $\lambda \to 0$, it can be shown that

$$\exp(-S[w]) = \exp\bigg(- \int w(\partial_t^2 - \partial_{\mathbf{z}}^2 + m^2) w \, d\mathbf{z}dt \bigg),$$

where Stokes theorem was used and the term on the boundary of (sample) space is set to zero. The above integral in the exponent is quadratic in w and the integral over $\mathcal{D}w$ can be done in a similar manner to Gaussian integrals. The correlation function of the fields across two points in space and time is

$$\langle w(\mathbf{z}_1, t_1) w(\mathbf{z}_2, t_2)\rangle = G(\mathbf{z}_1, t_1, \mathbf{z}_2, t_2),$$

where $G(\mathbf{z}_1, t_1, \mathbf{z}_2, t_2)$ is the Green's function to the Klein-Gordon equation, satisfying

$$(\partial_t^2 - \partial_{\mathbf{z}}^2 + m^2) G(\mathbf{z}_1, t_1, \mathbf{z}_2, t_2) = \delta(\mathbf{z}_1 - \mathbf{z}_2)\delta(t_1 - t_2).$$

The Fourier transformation of the correlation function is

$$G(\omega, \mathbf{k}) = \frac{1}{\omega^2 - |\mathbf{k}|^2 - m^2}, \quad m^2 > 0.$$

An inverse transform over ω gives

$$G(t, \mathbf{k}) = \frac{i}{2\omega_0} e^{-i\omega_0 t},$$

with $\omega_0^2 = |\mathbf{k}|^2 + m^2$.

C Spontaneous Symmetry Breaking in the Orthogonal Group O(D')

In this section we show that weights π with small, near zero, eigenvalues $m_\pi^2 = \frac{1}{4}\lambda\eta^2$ are generated by spontaneous symmetry breaking. Note that we can write the Lagrangian in Equation (2) as $\mathcal{L} = \mathcal{T} - \mathcal{V}$. Consider weights γ that transforms under O(D'), from Equation (2)

$$\begin{aligned} \mathcal{T} &= \frac{1}{2}(\partial_t \gamma^i)^2 - \frac{1}{2}(\partial_{\mathbf{z}} \gamma^i)^2, \\ \mathcal{V} &= \frac{m^2}{2}\gamma^i\gamma_i + \frac{\lambda}{4}(\gamma^i\gamma_i)^2. \end{aligned} \tag{4}$$

When $m^2 = -\mu^2 + \frac{1}{4}\lambda\eta^2 < 0$, it can be shown that in this case the loss minimum is no longer at $\gamma^i = 0$, but it has a degenerate minima on the surface such that $\sum_i (\gamma_i)^2 = v$, where $v = \sqrt{-m^2/\lambda}$. Now we pick a point on this loss minima and expand around it. Write $\gamma^i = (\pi^k, v + \sigma)$, where $k \in \{1, \ldots, D' - 1\}$. Intuitively, the π^k fields are in the subspace of degenerate minima and σ is the field orthogonal to π. Then it can be shown that the Lagrangian can be written as

$$\mathcal{L} = \mathcal{T}_\pi + \mathcal{T}_\sigma - \mathcal{V}_\pi - \mathcal{V}_\sigma - \mathcal{V}_{\pi\sigma},$$

where, in the weak coupling limit $\lambda \to 0$,

$$\begin{aligned}
\mathcal{T}_\pi &= \frac{1}{2}(\partial_t \pi^k)^2 - \frac{1}{2}(\partial_{\mathbf{z}} \pi^k)^2, \\
\mathcal{T}_\sigma &= \frac{1}{2}(\partial_t \sigma)^2 - \frac{1}{2}(\partial_{\mathbf{z}} \sigma)^2, \\
\mathcal{V}_\pi &= O(\lambda), \\
\mathcal{V}_\sigma &= -\frac{1}{2} m^2 \sigma^2, \\
\mathcal{V}_{\pi\sigma} &= O(\lambda),
\end{aligned} \tag{5}$$

the fields π and σ decouple from each other and can be treated separately. The σ fields satisfy the Klein-Gordon Equation $(\Box - m^2)\sigma = 0$, with $\Box = \partial_t^2 - \partial_{\mathbf{z}}^2$. The π fields satisfy the wave-equation, $\Box \pi = 0$. The correlation functions of the weights across sample space and layers, $P_\sigma = \langle \sigma(\mathbf{z}', t')\sigma(\mathbf{z}, t)\rangle$ and $P_\pi = \langle \pi(\mathbf{z}', t')\pi(\mathbf{z}, t)\rangle$ are the Green's functions of the respective equations of motion. Fourier transforming the correlation functions give

$$P_{\sigma,\pi}(t, \mathbf{k}) = \frac{i}{2\omega_0} \exp\Big(- i\omega_0 t \Big), \tag{6}$$

where $\omega_0 = \sqrt{|\mathbf{k}|^2 + |m^2_{\sigma,\pi}|}$, and $m^2_\pi = \frac{1}{4}\lambda\eta^2 \simeq 0$. The correlation function P_π is dominated by values of $|\mathbf{k}| \simeq 0$. Therefore $\langle \pi\pi \rangle \to \infty$ as $\lambda\eta^2 \to 0$. On the other hand, it can be shown that $\langle \sigma\sigma \rangle$ is damped by the weight eigenvalues $|m^2|$. The singularity in the correlation function means that the value of the weights at the start of the layer is highly correlated with the ones in later layers.

In the language of group theory. The O(D) symmetry is broken down to O($D-1$). Elements of O(D) are the $D \times D$ orthogonal matrices, which have $D(D-1)/2$ independent continous symmetries (e.g. the Euler angles in $D = 3$). The number of continuous broken from O(D) to O($D-1$) is $D-1$. In the above example we showed that this corresponds to the $D-1$ π^k fields. Each of which have zero Hessian eigenvalue.

Even though we formulated our field theory based on the decoupling limit of ResNets, the result of infinite correlation is very general and can be applied even if the decoupling limit is not valid. It is a direct result of spontaneous symmetry breaking. We state the Goldstone Theorem without proof.

Theorem (Goldstone): For every continuous symmetry that is spontaneously broken, a weight π with zero Hessisn eigenvalue is generated at zero temperature (learning rate η). $\Box$

D WHY GO QUANTUM?

In brief, the formulism for spontaneous symmetry breaking is mostly done in quantum field theory. We also believe that it is a good approximation to deep neural networks in the presence of the non-linear operators. The non-linear operators quantizes the input. For sigmoid, the output is $\{0, +1\}$ for the most part. And the negative end of ReLU is zero. The key is the discreteness in the difference between the input and output through the non-linearity. This discreteness assists the network to get to point A to C in Figure 1. Recall that we assume the layers are decoupled, which means that each layers have approximately the same distribution of weights. Suppose that the weights are now at A for all layers. Even if the learning rate is too small and the weights are stuck at A, the non-linearity knocks the weight in the next layer off A to give stochastic gradient descent a larger probability to reach C. Further, the action of non-linearities seems to be quantized in the frequency domain (Vasilyev, 2015) for a sine wave input.

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