Signal propagation in continuous approximations of binary neural networks

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Abstract

The training of stochastic neural network models with binary (±1) weights and activations via a deterministic and continuous surrogate network is investigated. We derive, using mean field theory, a set of scalar equations describing how input signals propagate through the surrogate network. The equations reveal that these continuous models exhibit an order to chaos transition, and the presence of depth scales that limit the maximum trainable depth. Moreover, we predict theoretically and confirm numerically, that common weight initialization schemes used in standard continuous networks, when applied to the mean values of the stochastic binary weights, yield poor training performance. This study shows that, contrary to common intuition, the means of the stochastic binary weights should be initialized close to ±1 for deeper networks to be trainable.

1. Introduction

Recent work in deep learning has used a mean field formalism to explain the empirically well known impact of initialization on the dynamics of learning (Saxe et al., 2013), (Poole et al., 2016), (Schoenholz et al., 2016). From one perspective (Poole et al., 2016), (Schoenholz et al., 2016), the formalism studies how signals propagate forward and backward in wide, random neural networks, by measuring how the variance and correlation of input signals evolve from layer to layer, knowing the distributions of the weights and biases of the network. By studying these moments the authors in (Schoenholz et al., 2016) were able to explain how heuristic initialization schemes avoid the “vanishing and exploding gradients problem” (Glorot & Bengio, 2010), establishing that for neural networks of arbitrary depth to be trainable they must be initialized at “criticality”, which corresponds to initial correlation being preserved to any depth.

Unfortunately, comparisons are difficult to make, since different algorithms may perform better under specific combinations of optimisation algorithms, initialisations, and heuristics such as drop out and batch normalization. Therefore a theoretical understanding of the various components of the algorithms is desirable. To date, the initialisation of any binary neural network algorithm has not been studied. Since all approximations still retain the basic neural network structure of layerwise processing, crucially applying backpropagation for optimisation, it is reasonable to expect that signal propagation will also be an important concept for these methods.

The continuous surrogate model of binary networks that we study makes use of the application of the central limit theorem (CLT) at the receptive fields of each neuron, assuming the binary weights are stochastic. Specifically, the fields are written in terms of the continuous means of stochastic binary weights, but with more complicated expressions than for standard continuous networks. The ideas behind the approximation are old (Spiegelhalter & Lauritzen, 1990) but have been renewed use in the current context from Bayesian (Ribeiro & Opper, 2011) (Hernández-Lobato & Adams, 2018).
We show that in this case the derivative calculated is only
with strongly broken symmetry, close to
and other important questions, in the discussion.

2. Background

2.1. Continuous neural networks and approximations
to binary networks

A neural network model is typically defined as a determinis-
tic non-linear function. We consider a fully connected
feedforward model, which is composed of \( N^\ell \times N^\ell-1 \)
weight matrices \( W^\ell \) and bias vectors \( b^\ell \) in each layer
\( \ell \in \{0, \ldots, L\} \), with elements \( W^\ell_{ij} \in \mathbb{R} \) and \( b^\ell \in \mathbb{R} \). Given
an input vector \( x^0 \in \mathbb{R}^{N_0} \), the network is defined in terms of
the following vector equations,

\[
x^\ell = \phi^\ell(h^\ell_{\text{ct}}), \quad h^\ell_{\text{ct}} = W^\ell x^{\ell-1} + b^\ell
\]

where the pointwise non-linearity is, for example, \( \phi^\ell(\cdot) = \tanh(\cdot) \). We refer to the input to a neuron, such as \( h^\ell_{\text{ct}} \), as
the pre-activation field.

In the binary neural network model that we study, we
instead have stochastic binary weight matrices and neu-
rons. We denote the matrices as \( S^\ell \) with all weights
\( S^\ell_{ij} \in \{\pm 1\} \) being independently sampled Bernoulli vari-
ables: \( S^\ell_{ij} \sim \text{Bernoulli}(M^\ell_{ij}) \), where the probability
of flipping is controlled by the mean \( M^\ell_{ij} := \mathbb{E}S^\ell_{ij} \). The
neurons in this model are also Bernoulli variables, controlled
by the incoming field \( h^\ell_{\text{sb}} = S^\ell x^{\ell-1} + b^\ell \) (SB denoting
"stochastic binary"). The idea behind several recent papers
(Soudry et al., 2014) (Baldassi et al., 2018), (Shayer et al.,
2017), (Peters & Welling, 2018) is to adapt the mean of
the Bernoulli weights, with the stochastic model essentially
used to "smooth out" the discrete variables and arrive at a
differentiable function, open to the application of continuous
optimisation techniques.

The algorithm we study here takes the limit of large layer
width to model the field \( h^\ell_{\text{sb}} \) as a Gaussian, with mean
\( \bar{h}^\ell := \sum_j M^\ell_{ij} x^{\ell-1}_j + b^\ell \) and variance \( \Sigma^\ell_{ij} = \sum_j 1 - (M^\ell_{ij} - x^{\ell-1}_j)^2 \).
This is the first level of mean field theory, which we can
apply successively from layer to layer by propagating means
and variances to obtain a differentiable, deterministic func-
tion of the \( M^\ell_{ij} \). Briefly, the algorithm can be derived as
follows. For a finite dataset \( D = \{x_\mu, y_\mu\} \), with \( y_\mu \) the
label, we define a cost via

\[
\mathcal{L}(f; M, b) = \sum_{\mu \in D} \log \mathbb{E}_{S,x}[p(y_\mu = f(x_\mu; S, b, x))]
\]

with the expectation \( \mathbb{E}_{S,x}[\cdot] \) over all weights and neurons.
This objective might also be recognised as a marginal like-
lihood, and so it is reasonable to describe this method as
Type II maximum likelihood, or empirical Bayes. In any
any, it is possible to take the expectation via approximate
analytic integration, leaving us with a completely deter-
ministic neural network with \( \tanh(\cdot) \) non-linearities, but
with more complicated pre-activation fields than a standard
neural network.

The starting point for this approximation comes from rewriting
the expectation \( \mathbb{E}_{S,x}[p(y_\mu = f(x_\mu; S, b, x))] \) in terms of
nested conditional expectations, similarly to a Markov
chain, with layers corresponding to time indices,

\[
\mathbb{E}_{S,x}[p(y_\mu = f(x_\mu; S, b, x))] = \sum_{s^\ell \in \mathbb{R}^{L+1}} \prod_{\ell=0}^{L-1} \sum_{x^\ell} \mathbb{E}_{S^\ell}[p(y_\mu = f(x_\mu; S, b, x))] = \sum_{s^L \in \mathbb{R}^{L+1}} \prod_{\ell=0}^{L-1} \sum_{x^\ell} \mathbb{E}_{S^\ell}[p(y_\mu = f(x_\mu; S, b, x))]\]

(3)

1 We follow the convention in physics models for 'spin' sites
\( S^\ell_{ij} \in \{\pm 1\} \), and also denote a stochastic binary
random variable with bold font.
Signal propagation in continuous approximations of binary neural networks

with the distribution of neurons factorising across the layer, given the previous layer, \( p(x_{l+1}^{\ell+1}|x^\ell) = \prod_i p(x_{l+1}^{\ell+1} | x^\ell_i, S^\ell_i) \).

The basic idea is to successively marginalise over the stochastic inputs to each neuron, calculating an approximation of each neuron’s probability distribution, \( \hat{p}(x^\ell_i) \). For Bernoulli neurons, the approximation is the well known Gaussian integral of the logistic sigmoid \(^{(Spiegelhalter & Lauritzen, 1990)}\) (see also \(^{(Crooks, 2013)}\))

\[
p(x^\ell_i) = \sum_{x^\ell_{i-1}} \sum_S p(x^\ell_i|x^\ell_{i-1}, S^\ell)p(S^\ell-1)\hat{p}(x^\ell_i) \\
\approx \int_{h^\ell_i} \sigma(h^\ell_i x^\ell_{i+1}) N(h^\ell_i | \bar{h}^\ell_i, (\Sigma_{MF})_{ii}) \\
\approx \sigma(\kappa (\Sigma_{MF})_{ii}^{-1/2} x^\ell_i) := \hat{p}(x^\ell_i) \tag{4}
\]

with \( \kappa = \sqrt{\frac{2}{\pi}} \) as a constant of the approximate integration \(^{(Crooks, 2013)}\), and where \( \Sigma_{MF} \) is the mean field approximation to the covariance between the stochastic binary pre-activations,

\[
(\Sigma_{MF})_{ij} = Cov(h^\ell_{SB}, h^\ell_{SB})_{ij} \delta_{ij} \tag{5}
\]

that is, a diagonal approximation to the full covariance (\( \delta_{ij} \) is the Kronecker delta). This approximate probability is then used as part of the Gaussian CLT applied at the next layer.

Given the approximately analytically integrated loss function, it is possible to perform gradient descent with respect to the \( M^\ell_i \) and \( b^\ell_i \). Importantly, we can write out the network forward equations analogously to the continuous case,

\[
x^\ell_i = \phi^\ell(\kappa h^\ell_i), \quad h^\ell = \sum_{a=1}^A \Sigma_{MF} a h^\ell_a, \quad \bar{h}^\ell = M^\ell x^\ell_{i-1} + b^\ell \tag{6}
\]

We note that the backpropagation algorithm derived in \(^{(Soudry et al., 2014)}\) was derived from a Bayesian message passing scheme, but removes all cavity arguments without corrections. As we have shown this algorithm is easier to derive from an empirical Bayes or maximum marginal likelihood formulation. Furthermore, in \(^{(Soudry et al., 2014)}\) the authors chose not to “backpropagate through” the variance terms, based on Taylor approximation and large layer width arguments. Results reported in \(^{(Baldassi et al., 2018)}\) utilise the complete chain rule but has not been applied to larger datasets than MNIST. We expand on this point in the discussion, when we consider the practical insights provided by the theory developed in this paper.

We should also remark that although \(^{(Shayer et al., 2017)}\), \(^{(Peters & Welling, 2018)}\) model the stochastic field \( h^\ell_{SB} \) as Gaussian (though in the former the activations are not stochastic), the authors utilise the local reparameterisation trick \(^{(Kingma & Welling, 2013)}\) to obtain differentiable networks. The resulting networks are not deterministic and even more significantly the backpropagation expressions fundamentally different to the algorithm studied here.

Accepting the definition \(^{(6)}\) of the forward propagation of an input signal \( x_0 \), we now move on to a second level of mean field, to study how a signal propagates on average in these continuous models, given random initialisation of the \( M^\ell \) and \( b^\ell \). This is analogous to the approach of \(^{(Poole et al., 2016)}\) who studied random \( W^\ell \) and \( b^\ell \) in the standard continuous case. The motivation for considering this perspective is that, despite having a very different pre-activation field, the surrogate model still maintains the same basic architecture, as seen clearly from the equations in \(^{(6)}\), and therefore is likely to inherit the same “training problems” of standard neural networks, such as the vanishing and exploding gradient problems \(^{(Glorot & Bengio, 2010)}\). Since the dynamic mean field theory of \(^{(Poole et al., 2016)}\) provides a compelling explanation of the dynamics of the early stages of learning, via signal propagation, it is worthwhile to see if this theory can be extended to the non-standard network definition in \(^{(6)}\).

2.2. Forward signal propagation for standard continuous networks

We first recount the formalism developed in \(^{(Poole et al., 2016)}\). Assume the weights of a standard continuous network are initialised with \( W^\ell_i \sim N(0, \sigma^2_\ell) \), biases \( b^\ell \sim N(0, \sigma^2_b) \), and input signal \( x^0_0 \) has zero mean \( \mathbb{E}x^0 = 0 \) and variance \( \mathbb{E}[x^0_i \cdot x^0_a] = q^0_{aa} \), and with \( a \) denoting a particular input pattern. As before, the signal propagates via equation \(^{(1)}\) from layer to layer.

The particular mean field approximation used here replaces each element in the pre-activation field \( h^\ell_i \) by a Gaussian random variable whose moments are matched. So we are interested in computing, from layer to layer, the variance \( q^\ell_{aa} = \frac{1}{N^\ell} \sum_i (h^\ell_{ia})^2 \) from a particular input \( x^0_a \), and also the covariance between the pre-activations \( q^\ell_{ab} = \frac{1}{N^\ell} \sum_i h^\ell_{ia} h^\ell_{ib} \), arising from two different inputs \( x^0_a \) and \( x^0_b \) with given covariance \( q^0_{ab} \). As explained in \(^{(Poole et al., 2016)}\), assuming the independence within a layer; \( \mathbb{E}h^\ell_{ia}h^\ell_{ja} = q^\ell_{aa} \delta_{ij} \) and \( \mathbb{E}h^\ell_{ia} h^\ell_{jb} = q^\ell_{ab} \delta_{ij} \), it is possible to derive recurrence rela-
tions from layer to layer
\[ q_{\ell a}^t = \sigma^2_w \int Dz \phi^2(\sqrt{q_{\ell a}^t} z) + \sigma^2_b \]
\[ := \sigma^2_w E \phi^2(h_{j,a}^{\ell-1}) + \sigma^2_b \]  
(7)

with \( Dz = \frac{dz}{\sqrt{2\pi}} e^{-z^2/2} \) the standard Gaussian measure. The recursion for the covariance is given by
\[ q_{\ell b}^t = \sigma^2_w \int Dz_1 Dz_2 \phi(u_a)\phi(u_b) + \sigma^2_b \]
\[ := \sigma^2_w E \phi(h_{j,a}^{\ell-1})\phi(h_{j,b}^{\ell-1}) + \sigma^2_b \]  
(8)

where
\[ u_a = \sqrt{q_{\ell a}^{t-1}} z_1, \quad u_b = \sqrt{q_{\ell b}^{t-1}} (\epsilon_{b}^{\ell-1} z_1 + \sqrt{1 - (\epsilon_{b}^{\ell-1})^2} z_2) \]

and we identify \( \epsilon_{ab}^{\ell} \) as the correlation in layer \( \ell \). Arguably the most important quantity is the slope of the correlation recursion equation or mapping from layer to layer, denoted as \( \chi \), which is given by:
\[ \chi = \frac{\partial \epsilon_{ab}^{\ell}}{\partial \epsilon_{ab}^{\ell-1}} = \sigma^2_w \int Dz_1 Dz_2 \phi^2(u_a)\phi(u_b) \]  
(9)

As discussed (Poole et al., 2016), when \( \chi_{c*} = 1 \) the system is at a critical point where correlations can propagate to arbitrary depth, corresponding to the edge of chaos. In continuous networks, \( \chi \) is equivalent to the mean square singular value of the Jacobian matrix for a single layer \( J_{ij} = \frac{\partial h_i^{\ell}}{\partial h_j^{\ell}} \), as explained in (Poole et al., 2016). Therefore controlling \( \chi \) will prevent the gradients from either vanishing or growing exponentially with depth.

In (Schoenholz et al., 2016) explicit depth scales for standard neural networks are derived, which diverge corresponding when \( \chi_{c*} = 1 \), thus providing the bounds on maximum trainable depth. We will not rewrite these continuous depth scales, since these resemble those in the Gaussian-binary case with which we now proceed.

3. Theoretical results

3.1. Forward signal propagation for deterministic Gaussian-binary networks

For the Gaussian binary model we assume means initialised from some bounded distribution \( M_{ij}^\ell \sim P(M = M_{ij}) \), with mean zero and variance of the means \( \sigma^2_m \). For instance, a valid distribution could be a clipped Gaussian,\(^3\) or another Bernoulli, for example \( P(M) = \frac{1}{2} \delta(M = +\sigma_m) + \frac{1}{2} \delta(M = -\sigma_m) \), whose variance is \( \sigma^2_m \). The biases are distributed as \( b^\ell \sim \mathcal{N}(0, N_{2d-1} \sigma^2_b) \), with the variance scaled by the previous layer width \( N_{2d-1} \) since the denominator of the pre-activation scales with \( N_{2d-1} \) as seen from the definition (6). Once again we have input signal \( x_0^\ell \), with zero mean \( E x_0^\ell = 0 \), and with a denoting a particular input pattern. Assume a stochastic neuron with mean \( x^\ell_i := E_{p(x)} x_i^\ell = \phi(h_{i}^{\ell-1}) \), where the field is once again given by:
\[ h_{i}^{\ell} = \frac{\sum_j M_{ij}^\ell \phi(h_{j}^{\ell-1}) + b_i^\ell}{\sqrt{\sum_j [1 - (M_{ij}^\ell)^2 \phi^2(h_{j}^{\ell-1})]}} \]  
(10)

which we can read from the vector equation (6). Note in the first layer the denominator expression differs since in the first level of mean field analysis the inputs are not considered random (since we are in a supervised learning setting, see supplementary material (SM, 2019)). As in the continuous case we are interested in computing the variance \( q_{aa}^{\ell} = \frac{1}{N} \sum_j (h_{j,a}^{\ell})^2 \) and covariance \( \text{E}(h_{i}^{\ell}, h_{j}^{\ell}) = q_{ab}^{\ell} \delta_{ij} \), via recursive formulæ. The key to the derivation is recognising that the denominator is a self-averaging quantity,
\[ \lim_{N \to \infty} \frac{1}{N} \sum_j 1 - (M_{ij}^\ell)^2 \phi^2(h_{j}^{\ell-1}) = 1 - E[(M_{ij}^\ell)^2 \phi^2(h_{j}^{\ell-1})] \]  
(11)
\[ = 1 - \sigma^2_m E \phi^2(h_{j}^{\ell-1}) \]  
(12)
\[ = 1 - \sigma^2_m \text{var}(h_{j}^{\ell-1}) \]  
(13)

where we have used the properties that the \( M_{ij}^\ell \) and \( h_{j}^{\ell-1} \) are each i.i.d. random variables at initialisation, and independent (Mezard et al., 1987). Following this self-averaging argument, we can take expectations more readily as shown in the supplementary material (SM, 2019), finding the variance recursion
\[ q_{aa}^{\ell} = \frac{\sigma^2_m \text{var}(h_{j}^{\ell-1}) + \sigma^2_b}{1 - \sigma^2_m \text{var}(h_{j}^{\ell-1})} \]  
(14)

and then based on this expression for \( q_{aa}^{\ell} \), and assuming \( q_{bb}^{\ell} = q_{bb} \), the correlation recursion can be written as
\[ \epsilon_{ab}^{\ell} = \frac{1 + q_{aa}^{\ell} \sigma^2_m \text{var}(h_{j}^{\ell-1}) + \sigma^2_b}{1 + \sigma^2_b} \]  
(15)

The slope of the correlation mapping from layer to layer, when the normalized length of each input is at its fixed point \( q_{aa}^{\ell} = q_{bb} \), is given by:
\[ \chi = \frac{\partial \epsilon_{ab}^{\ell}}{\partial \epsilon_{ab}^{\ell-1}} = \frac{1 + q^* \sigma^2_m}{1 + \sigma^2_b} \int Dz_1 Dz_2 \phi(u_a)\phi(u_b) \]  
(16)

where \( u_a \) and \( u_b \) are defined exactly as in the continuous case. Refer to the supplementary material (SM, 2019) for full details of the derivation. The recursive equations derived for this model and the continuous neural network are qualitatively similar, and by observation allow for the calculation of depth scales, just as in the continuous case (Schoenholz et al., 2016).
3.2. Asymptotic expansions and depth scales

In the continuous case, when \( \chi \) approaches 1, we approach criticality and the rate of convergence to any fixed point slows. The depth scales, as derived in (Schoenholz et al., 2016) provide a quantitative indicator to the number of layers correlations will survive for, and thus how trainable a network is. We show here that similar depth scales can be derived for these Gaussian-binary networks.

According to (Schoenholz et al., 2016) it should hold asymptotically that \( |q^\ell_{aa} - q^*| \sim \exp(-\frac{\ell}{\xi_q}) \) and \( |c^\ell_{ab} - c^*| \sim \exp(-\frac{\ell}{\xi_c}) \) for sufficiently large \( \ell \) (the network depth), where \( \xi_q \) and \( \xi_c \) define the depth scales over which the variance and correlations of signals may propagate. Writing \( q^\ell_{aa} = q^* + \epsilon^\ell \), we can show that (SM, 2019):

\[
\epsilon^{\ell+1} = \frac{\epsilon^\ell}{1 + q^*} \left[ \chi_1 + \frac{1 + q^*}{1 + \sigma_b^2} \int Dz \phi''(\sqrt{q^*}z)\phi(\sqrt{q^*}z) \right] + \mathcal{O}(\epsilon^{2\ell})
\]

(17)

We can similarly expand for the correlation \( c^\ell_{ab} = c^* + \epsilon^\ell \), and if we assume \( q^\ell_{aa} = q^* \), we can write

\[
\epsilon^{\ell+1} = \frac{\epsilon^\ell}{1 + \sigma_b^2} \left[ \frac{1 + q^*}{2} \int Dz \phi''(u_1)\phi'(u_2) \right] + \mathcal{O}(\epsilon^{2\ell})
\]

(18)

The depth scales we are interested in are given by the log ratio \( \log \frac{\ell+1}{\epsilon} \).

\[
\xi_q^{-1} = \log(1 + q^*) - \log \left[ \chi_1 + \frac{1 + q^*}{1 + \sigma_b^2} \int Dz \phi''(\sqrt{q^*}z)\phi(\sqrt{q^*}z) \right]
\]

(19)

\[
\xi_c^{-1} = -\log \left[ \frac{1 + q^*}{1 + \sigma_b^2} \int Dz \phi''(u_1)\phi'(u_2) \right] = -\log \chi
\]

(20)

The arguments used in the original derivation (Schoenholz et al., 2016) carry over to the Gaussian-binary case in a straightforward manner, albeit with more tedious algebra.

3.3. Jacobian mean squared singular value and Mean Field Gradient Backpropagation

As mentioned in the introduction, an equivalent perspective on this work is that we are simply attempting to control the mean squared singular value of the input-output Jacobian matrix of the entire network, which we can decompose into the product of single layer Jacobian matrices,

\[
J = \prod_{\ell=1}^{L} J^\ell, \quad J^\ell_{ij} = \frac{\partial h^\ell_{i,j,a}}{\partial h^\ell_{j,a}}
\]

(21)

In standard networks, the single layer Jacobian mean squared singular value is equal to the derivative of the correlation mapping \( \chi \) as established in (Poole et al., 2016),

\[
\left\langle \frac{||J'_{u}||^2_2}{||u||^2_2} \right\rangle = \chi
\]

(22)

where we average over the weights, Gaussian distribution of \( h^\ell_{i,j,a} \) and the random perturbation \( u \). For the Gaussian model studied here this is not true, and corrections must be made to calculate the true mean squared singular value. This can be seen by observing the terms arising from denominator of the pre-activation field\(^4\),

\[
J^\ell_{ij} = \frac{\partial h^\ell_{i,j,a}}{\partial h^\ell_{j,a}} = \frac{\partial}{\partial h^\ell_{j,a}} \left( \frac{h^\ell_{i,j,a}}{\sqrt{\Sigma_{ii}}} \right)
\]

\[
= \phi'(h^\ell_{i,j,a}) \left[ \frac{M^\ell_{ij}}{\Sigma_{ii}} + (M^\ell_{ij})^2 \frac{\bar{h}_{i,a}^\ell}{(\Sigma_{ii})^{1/2}} \phi(h^\ell_{i,a}) \right]
\]

(23)

Since \( \Sigma_{ii} \) is a quantity that scales with the layer width \( N_i \), it is clear that when we consider squared quantities, such as the mean squared singular value, the second term, from the derivative of the denominator, will vanish in the large layer width limit. Thus the mean squared singular value of the single layer Jacobian approaches \( \chi \). We now proceed as if \( \chi \) is the exact quantity we are interested in controlling.

The analysis involved in determining whether the mean squared singular value is well approximated by \( \chi \) essentially takes us through the mean field gradient backpropagation theory as described in (Schoenholz et al., 2016). This idea provides complementary depth scales for gradient signals travelling backwards. We now move on to simulations of random networks, verifying that the theory accurately predicts the average behaviour of randomly initialised networks.

3.4. Simulations

We see in Figure 1 that the average behaviour of random networks are well predicted by the mean field theory. The estimates of the variance and correlation from simulations of random neural networks provided some input signals are plotted. The dotted lines correspond to empirical means, the shaded area corresponds to one standard deviation, and solid lines are the theoretical prediction. We see strong agreement in both the variance and correlation plots.

Finally, in Figure 2 we present the variance and correlation depth scales as a function of \( \sigma_m \), and different curves corresponding to different bias variance values \( \sigma_b \). We see that just as in continuous networks, \( \sigma_b \) and \( \sigma_m \) compete to effect the depth scale, which only diverges with \( \sigma_m \rightarrow 1 \). We notice that contrary to standard networks where \( \sigma_b \) is scaled

\(^4\)We drop the ‘mean field’ notation from \( \Sigma_{MF} \) for simplicity.
within one order of magnitude, that \( \sigma_b \) must be changed across orders of magnitude to produce an effect, due to the scaling with the width of the network. Importantly, we notice that the depth scale only diverges at one value for \( \sigma_m^2 \) (ie. at one), whereas for continuous networks there are an infinite number of such points.

3.5. Remark: Validity of the CLT for the first level of mean field

A legitimate immediate concern with initialisations that send \( \sigma_m^2 \to 1 \) may be that the binary stochastic weights \( S_{ij}^f \) are no longer stochastic, and that the variance of the Gaussian under the central limit theorem would no longer be correct. First recall the CLT’s variance is given by \( \text{Var}(h_{SB}^f) = \sum_j (1 - m_j^2 x_j^2) \). If the means \( m_j \to \pm 1 \) then variance is equal in value to \( \sum_j m_j^2 (1 - x_j^2) \), which is the central limit variance in the case of only Bernoulli neurons at initialisation. Therefore, the applicability of the CLT is invariant to the stochasticity of the weights. This is not so of course if both neurons and weights are deterministic, for example if neurons are just \( \tanh() \) functions.

4. Experimental results

4.1. Training performance for different mean initialisation \( \sigma_m^2 \)

Here we test experimentally the predictions of the mean field theory by training networks to overfit a dataset in the supervised learning setting, having arbitrary depth and different initialisations. We use the MNIST dataset with reduced training set size (25%) and record the training performance (percentage of the training set correctly labeled) after 20 epochs of gradient descent over the training set, for various network depths \( L < 100 \) and different mean variances \( \sigma_m^2 \in [0, 1] \). The optimizer used was Adam (Kingma & Ba, 2014) with learning rate of \( 2 \times 10^{-4} \) chosen after simple grid search, and a batch size of 64.

We see that the experimental results match the correlation depth scale derived, with a similar proportion to the standard continuous case of \( 6\xi_c \) being the maximum possible attenuation in signal strength before trainability becomes difficult, as described in (Schoenholz et al., 2016).

The reason we see the trainability not diverging in Figure 3 is that training time increases with depth, on top of requiring smaller learning rates for deeper networks, as described in detail in (Saxe et al., 2013). The experiment here used the same number of epochs regardless of depth, meaning shallower networks actually had an advantage over deeper networks, and yet still we see the initial variance \( \sigma_m^2 \) overwhelmingly the determining factor for trainability.

We notice a slight drop in trainability as the variance \( \sigma_m^2 \) approaches very close to one, as argued previously we do not believe this to be due to violating the CLT at the first level of mean field theory, however the input layer neurons are deterministic, so this may be an issue in the first CLT.

Another possibility is that if \( \sigma_m^2 \) gets very close to one, the algorithm may be frozen in a poor initial state.

We should note that this theory does not specify for how many steps of training the effects of the initialisation will persist, that is, for how long the network remains close to criticality. Therefore, the number of steps we trained the network for is an arbitrary choice, and thus the experiments validate the theory in a more qualitative than quantitative way. Results were similar for other optimizers, including SGD, SGD with momentum, and RMSprop. Note that these networks were trained without dropout, batchnorm or any other heuristics.

4.2. Test performance for different mean initialisation \( \sigma_m^2 \)

The theory we have presented relates directly to the ability for gradients to propagate backwards, in the same vein as (Schoenholz et al., 2016), and does not purport to relate
initialisation to generalisation performance. Of course, if a neural network is unable to memorise patterns from the training set at all, it is unlikely to generalise well.

We note that (Schoenholz et al., 2016) did not study or present test performance for standard networks, though for MNIST the scores obtained were reported to be at least 98%. Here we present the training and test results for the continuous surrogate network, for shallower networks \( L \leq 20 \), though still deeper than most binary neural networks. The reason we do this is to reveal a fundamental difference to standard continuous networks; we observe in Figure 4(b) the test performance increase with \( \sigma^2_m \) before decreasing as it approaches one.

Thus, we see an apparent conflict between trainability and generalisation, and possibly a fundamental barrier to the application of the algorithm (Baldassi et al., 2018), (Soudry et al., 2014). More generally, we note that such a tension between trainability and generalisation has not been observed in binary neural network algorithms to our knowledge, and seems to only have been speculated to occur in standard continuous neural networks recently (Advani & Saxe, 2017).

### 5. Discussion

In this paper we have theoretically studied binary neural network algorithms using dynamic mean field theory, following the analysis recently developed for standard continuous neural networks (Schoenholz et al., 2016). Based on self-averaging arguments, we were able to derive equations which govern signal propagation in wide, random neural networks, and obtained depth scales that limit trainability. This first study of a particular continuous surrogate network, has yielded results of practical significance, revealing that these networks have poor trainability when initialised away from \( \pm 1 \), as is common practice.

While we have focused on signal propagation, as a view towards controlling properties of the entire network’s Jacobian matrix, the generalisation ability of the algorithms developed is of obvious importance. The studies of the test performance reveal that the approach to criticality actually corresponds to a severe degradation in test performance.

It is possible that as \( \sigma^2_m \to 1 \) the ability for the gradient algorithm to shift the means from the initial configuration is hampered, as the solution might be frozen in this initial state. Another explanation can be offered however, by examining results for continuous networks. Recent theoretical work (Advani & Saxe, 2017) has established that initialising weights with small variance is fundamentally important for generalisation, which led to the authors to conclude with the open question,

“It remains to be seen how these findings might generalize to
deeper nonlinear networks and if the requirement for good generalization (small weights) conflicts with the requirement for fast training speeds (large weights, (Saxe et al., 2013)) in very deep networks.”

It is possible in the continuous surrogate studied here, it is this conflict that we observe. Perhaps surprisingly, we observe this phenomenon even for shallow networks.

Taking a step back, it might seem to the reader that the standard continuous networks and the continuous surrogate networks are remarkably similar, despite the latter being derived from an objective function with stochastic binary weights. Indeed, the similarities are of course what motivated this study; both can be described with via a set of recursive equations and have depth scales governing the propagation of signals. The obvious, and crucial, difference that we can extract directly from the mean field description of the surrogate network is that there is only one point at which the depth scale diverges. Furthermore, this occurs at the maximum of the means’ initial variance $\sigma_m^2 = 1$. By comparison, in standard continuous networks, there is no maximum variance, and in practice it is possible to achieve criticality for an initial variance small enough for generalisation to be easily achieved.

In its generality, this study appears to have revealed fundamental difficulties in the use of first order gradient descent to optimise this surrogate network, as derived from the original stochastic binary weight objective. Whether we can attribute this difficulty to the surrogate network itself, or whether it is the underlying binary or stochastic binary problem, is an open question.

We believe the work here is important for the development of binary neural network algorithms, several of which have opted to define stochastic binary networks as a means of smoothing out the non-differentiability (Baldassi et al., 2018), (Shayer et al., 2017), (Peters & Welling, 2018). It is a matter of future work to study these other algorithms, where the use of the self-averaging argument is likely to be the basis for deriving the signal propagation equations for these models.

This paper raises other open questions as well. In terms of further theoretical tools for analysis, the perspective of controlling the spectrum of input-output Jacobian matrix first proposed in (Saxe et al., 2013) is a compelling one, especially if we are interested purely in the optimisation of neural networks, since the spectral properties of the Jacobian matrix control much of the gradient descent process. This line of work has been extensively developed using random matrix theory in (Pennington et al., 2017) (Pennington et al., 2018), from the original proposals of (Saxe et al., 2013) regarding orthogonal initialisation, which allows for large training speed gains. For example, orthogonal initialisations were recently defined for convolutional neural networks, allowing for the training of networks with tens of thousands of layers (Xiao et al., 2018). Whether a sensible orthogonal initialisation can be defined for binary neural network algorithms, and if it is possible to apply the random matrix calculations are important questions, with the study here providing an natural first step.

Finally we note that these results may be of interest to researchers of Bayesian approaches to deep learning, since the deterministic Gaussian approximations presented here have been used as the basis of approximate variational Bayesian algorithms (Hernández-Lobato & Adams, 2015).
Signal propagation in continuous approximations of binary neural networks

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