
Meanfield theory of activation functions in Deep Neural Networks

Mirco Milletari¹ Thiparat Chotibut² Paolo E. Trevisanutto³

Abstract

We present a statistical mechanics model of deep neural networks, connecting the energy-based and the feed forward (FFN) approach. We infer that FFN can be understood as performing three basic steps: encoding, representation validation and propagation. From the meanfield solution of the model, we obtain a set of natural activations – such as sigmoid, tanh and ReLU – together with the state-of-the-art, Swish; this represents the expected information propagating through the network and tends to ReLU in the limit of zero noise. We study the spectrum of the Hessian on an associated classification task, showing that Swish allows for more consistent performances over a wider range of network architectures.

1. Introduction

Advances in modern computing hardware and availability of massive datasets have empowered multilayer artificial neural networks, or deep learning (DL), with unprecedented capabilities for image and speech recognition tasks. Despite these empirical success, theoretical understanding of why and when multilayer neural networks perform well lags far behind (Mézard, 2018). Only recently, theoretical efforts in this direction have been intensively reported. For example, recent works shed light on how FFN attains its expressive power (Poggio et al., 2017; Lin et al., 2017; Raghu et al., 2016; Poole et al., 2016), what contributes to its generalizability (Zhang et al., 2017; Dinh et al., 2017), and how myriad parameters in the network affect the geometry of the loss function (Dauphin et al., 2014; Choromanska et al., 2015; Pennington & Bahri, 2017; Pennington & Worah, 2017). Taken together, these theoretical results have paved the way for a systematic design of robust and explainable FFNs.

Using modern optimization and regularization techniques such as dropout (Srivastava et al., 2014), non-linear activation functions, and complex network architectures (Krizhevsky et al., 2012), to name a few, the

FFN can be efficiently trained on large-scale datasets such as ImageNet or CIFAR to achieve low training and generalization errors. While these engineering feats improve the performance of FFN, a clear design principle is still lacking, leading to an unsystematic growth of model complexity.

To assist future systematic studies and construction of FFNs, we propose a theoretical framework based on the tool-set of statistical mechanics. It allows for the definition of an energy based model in which a hidden unit is regarded as a communication channel, first encoding and then transmitting the result of its computation through a gate with a specific transmission probability; the latter is obtained via the maximum entropy principle (Nguyen et al., 2017; Jaynes, 2003) under the biologically inspired constraint that a neuron responds by firing (transmit its signals) or not with a certain probability. By interpreting a hidden unit as a communication channel, its activation takes the form of the expected (mean) signal transmission; remarkably, this activation corresponds to Swish, obtained in Ref. (Elfwing et al., 2014; Ramachandran et al., 2017) through an extensive search algorithm trained with reinforcement learning and shown to best perform on the CIFAR and ImageNet datasets among all candidate activations. Although some activations may perform better for the specific datasets they have been designed for, they generally fail to generalize. Finally, the standard ReLU activation arises as a limiting, noiseless case of Swish. To the best of our knowledge, this provides the first derivation of ReLU, typically introduced heuristically to facilitate optimization protocols. Despite restricting our analysis to pure FFNs, most of our conclusions carry on to Convolutional and Recurrent networks.

The paper is organized as follows: In 2, we provide a plausible argument based on dimensional analysis to explain why a hidden unit should be regarded as a communication channel. Following Refs. (Tishby & Zaslavsky, 2015; Schwartz-Ziv & Tishby, 2017), we show that each hidden unit acts first as an encoder and then as a filter determining the quality of its input. In 3, we explore the geometry of loss surfaces associated to Swish hidden units. The fraction of negative eigen-

values (α) of the Hessian (a measure of descent directions), as well as the fraction of zero eigenvalues, γ (a measure of flat directions), are investigated. We find that FFNs trained with ReLU always exhibit $\gamma \neq 0$ while those trained with Swish often show $\gamma \simeq 0$, resulting in faster and more flexible training. These two indices seem to determine not only the speed of learning but also whether this will be successful.

2. Motivation and Model

2.1. General Setup

A standard task in supervised learning is to determine an input/output relation between a set of m features and the observed labeled outcomes. Let us denote with x_i^μ the input vector, where $i \in [1, n]$ denotes a feature component, and $\mu \in [1, m]$ denotes an example; we also denote the output as y_k^μ , where k is the number of classes. Quite generally, the probability of measuring the output \mathbf{y} given the input can be written as $P(\mathbf{y}) = \int d\mathbf{x} P(\mathbf{y}|\mathbf{x}) P(\mathbf{x}) = \int d\hat{\mathbf{y}} P(\mathbf{y}|\hat{\mathbf{y}}) P(\hat{\mathbf{y}})$ where we have used the chain rule (A) and introduced the output layer ($\hat{\mathbf{y}}$). Once $P(\hat{\mathbf{y}})$ has been learned, one can obtain the loss function by taking the log-likelihood $\mathcal{L} = -\log P(\mathbf{y})$; for example, in a binary classification problem, $P(\hat{\mathbf{y}}[\theta])$ is Bernoulli and parametrized by $\theta_l = \{\mathbf{W}_l, \mathbf{b}_l\}$, being the weights and biases of the neural network, with $l \in [1, L]$ the number of hidden layers. In this case, the loss function is the binary cross-entropy, but other statistical assumptions lead to different Losses; see (A) for a meanfield derivation of the cross-entropy. To motivate the model, in the next section we begin by discussing a (physical) dimensional inconsistency in the standard formulation of forward propagation in FFNs, and how this can be reconciled within the proposed framework.

2.2. Motivations

Motivated by neurobiology and in analogy with the communication channel scheme in information theory (MacKay, 2003; Jaynes, 2003), we regard the input vector x_i^μ as the information source entering the processing units (neurons) of the network, while the units constitute the encoders. Quite generally, the encoders can either build a lower (compression) or higher dimensional (redundant) representation of the input data by means of a properly defined transition function. In a FFN, the former corresponds to a compression layer (fewer units) while the latter to an expansion layer (more units). If the encoded information constitutes an informative representation of the output signal (given the input), it is passed over to the next layer for further processing until the output layer

is reached. In the biological neuron, this last step is accomplished by the synaptic bouton, that releases information whether or not the input signal exceeds a local bias potential b_i . Both in the brain and in electronic devices, the input information is often conveyed in the form of an electric signal, with the electron charge being the basic unit of information, the signal has dimension (units) of *Coulomb* in SI. For an image, the information is the brightness level of each pixel, physically proportional to the current passing through it; on a computer, this is encoded in bits. Clearly, a linear combination of the input signals, together with the bias, has to preserve dimensions:

$$h_i^\mu = \sum_{j=1}^n w_{ij} x_j^\mu + b_i, \quad (1)$$

where $i \in [1, n_1]$ indices the receiving units in the first layer and the weight matrix w_{ij} is the coefficient of the linear combination and it is dimensionless.

For noiseless systems, the input is transmitted i.f.f. the overall signal exceeds the bias b_i . However, in the presence of noise, the signal can be transmitted with a certain probability even below the threshold; in the biological neuron, the variance in the number of discharged vesicles in the synaptic bouton and the number of neurotransmitters in each vesicle is responsible for such noisy dynamics (Amit, 1989). In so far, we just described the general functioning principle underlying FFNs. Let us first consider the sigmoid non-linearity $\sigma(\beta \mathbf{h})$, where β has inverse dimension of \mathbf{h} ; σ expresses the probability of the binary unit to be active (1) and can be seen as an approximation of the biological neuron's firing probability (Amit, 1989). Being a distribution defined in $[0, 1]$, σ is intrinsically dimensionless. The parameter β defines the spread of the distribution, tuning to the noise strength; typically, one sets $\beta = 1$ or reabsorb it inside the weights and bias (Nguyen et al., 2017), but here we keep it general for reasons that will be clear later. Defining $\mathbf{a} = \sigma(\beta \mathbf{h})$ as the input of the next layer, we can immediately see the dimensional mismatch: a linear combination of \mathbf{a} is dimensionless and when passed through the new non-linearity, $\sigma(\beta \mathbf{a})$ necessarily becomes dimensionful ($\beta \mathbf{a}$ now has dimension of noise). In the next section we show how this simple fact relates to gradients vanishing during back propagation. From a conceptual point of view, one is transmitting the expectation value of the transmission gate (synapse) rather than the processed signal. This problem persists when using the tanh activation, but it is absent when using ReLU, that correctly transmits the information itself.

2.3. Statistical mechanics of Feed Forward networks

A prototypical statistical mechanics formulation of Neural Networks is the inverse Ising problem (Nguyen et al., 2017), or Boltzmann machine, where one is interested in inferring the values of the couplings and external fields of the Ising model. While the Boltzmann machine is an energy-based model, standard FFN is not commonly regarded as such. Here, we propose to bridge on these two formulations using the maximum entropy principle (Nguyen et al., 2017; Di-Castro & Raimondi, 2003; MacKay, 2003; Jaynes, 2003) to obtain the least biased representation of hidden neurons. Starting from the input layer, each unit takes the same input vector \mathbf{x} and outputs a new variable \mathbf{h} . We now regard h_i as an effective, coarse grained field coupling to the synaptic gate variable s_i . The feedforward nature of coarse graining (a directed graph), stems from its irreversibility and endorses the forward pass with a semi-group structure. Considering the first layer, we need to evaluate the probability associated to the new, coarse grained variable \mathbf{h} , $P(\mathbf{h}) = \int d\mathbf{x} Q(\mathbf{h}|\mathbf{x}) P(\mathbf{x})$, where $Q(\mathbf{h}|\mathbf{x})$ is the transition function modelling the encoder. In DL, the latter is fixed by the forward pass, while the input data are drawn from some unknown distribution $P(\mathbf{x})$. We can follow two different paths: fix the value of \mathbf{x} on the observed (empirical) sequence, or assume the form of the distribution from which \mathbf{x} has been sampled from; here we choose the former option. Consider then the empirical estimator $P(\mathbf{x}) = \prod_{\mu=1}^m \delta(\mathbf{x} - \mathbf{x}^\mu)$, where the Dirac-delta function fixes the input on the observed sequence. As for the transition function, it enforces the information processing performed by the “soma” of the artificial neuron; in DL, this consists of creating a linear combination of the input information. Information conservation, enforces an additional constrain on the coefficients of the transformation, namely $\sum_i w_{ij}^{[l]} = 1 \forall l = 1, \dots, L$, formally equivalent to the conservation of charge in an electronic system and to an L_1 regularisation in DL:

$$P(\mathbf{h}) = \int d\mathbf{x} \Gamma^{[1]} \delta(\mathbf{h} - \mathbf{w}^T \mathbf{x} - \mathbf{b}) \prod_{\mu=1}^m \delta(\mathbf{x} - \mathbf{x}^\mu) \quad (2)$$

$$\Gamma^{[1]} = \prod_{j=1}^n \delta\left(\sum_{i=1}^{n_1} w_{ij}^{[1]} - 1\right).$$

The relation between DL and the renormalization group (RG) was previously observed in the context of restricted Boltzmann machine (RMB) (Mehta & Schwab, 2014); in A.b we show how this concept generalizes to FFN via Eq. (2).

Once \mathbf{h} has been computed, the information passes through the “synaptic” gate, and transmitted with a certain probability if it exceeds the threshold potential b_i . The core task at hand is to determine the state of the gate (open/close). The absence of lateral connections in FFNs means that each synaptic gate is only influenced by its receptive signal as the intralayer correlations are taken – a priori – to be zero. Given a statistical ensemble of hidden binary gates, the most likely distribution can be obtained by maximising its entropy, subject to constraints imposed by the conserved quantities, i.e. the first and second moments of the data (Nguyen et al., 2017; MacKay, 2003). However, in the absence of lateral connections, the entropy functional of the hidden gate s_i does not account for the second moment. Functionally varying with respect to the probability $P(\mathbf{s})$ and solving for the Lagrange multipliers, one obtains (Di-Castro & Raimondi, 2003):

$$P(\mathbf{s}|\mathbf{h}) = \frac{1}{Z} e^{\sum_i \beta_i s_i h_i} \quad (3)$$

$$Z[\mathbf{h}] = \prod_i \sum_{s_i \in \{0,1\}} e^{\beta_i s_i h_i} = \prod_i (1 + e^{\beta_i h_i}),$$

where β_i encodes the noise. In a physical system, β_i is the inverse temperature in units of Boltzmann’s constant and in equilibrium it is the same for each s_i ; however, here the network is only in a local equilibrium as the units are not allowed to exchange “energy” (information) among themselves due to the lack of pairwise interactions. We have introduced $P(\mathbf{s}|\mathbf{h})$ to denote the conditional probability of \mathbf{s} given the signal \mathbf{h} – and the partition function Z . Finally, given the distribution of the coarse grained inputs and the conditional probability of the channels $P(\mathbf{s}|\mathbf{h})$, one is left evaluating the channel transmission probability

$$P(\mathbf{s}) = \int d\mathbf{h} P(\mathbf{s}|\mathbf{h}) P(\mathbf{h}) = \frac{1}{Z} e^{-\sum_i \beta_i \mathcal{H}_i[s, \mathbf{x}^\mu]} \quad (4)$$

$$Z = \frac{1}{m} \prod_{\mu=1}^m \prod_{i=1}^{n_1} [1 + e^{\beta_i h_i^\mu}] = \frac{1}{m} \prod_{\mu=1}^m \prod_{i=1}^{n_1} Z_{i,\mu},$$

where $\hat{h}_i^\mu = \sum_j w_{ij}^{[1]} x_j^\mu + b_i$, $Z_{i,\mu}$ is the partition function per example/index and we have identified the simple coarse grained Hamiltonian $\mathcal{H}_i = -\sum_{j=1}^n s_i w_{ij}^{[1]} x_j^\mu - s_i b_i$. Eq. (4) is the starting point of an energy based model, where it is the coarse grained probability $P(\mathbf{s})$ that propagates through the network (see e.g. (Kou et al., 2018)) as opposed to signals in a FFN; indeed, the \mathcal{H} has the form of a RBM with binary hidden units. The expected value of the channel transmission, $\langle s_i \rangle$ is (Hertz et al., 1991) the logistic function, for each empirical realization μ

and unit i :

$$\langle s_i \rangle = \frac{1}{\beta_i} \frac{\partial}{\partial b_i} \log Z_{i,\mu} = \frac{1}{1 + e^{-\beta_i \hat{h}_i^\mu}} \equiv \sigma(\beta_i \hat{h}_i^\mu). \quad (5)$$

We stress that this is not the coarse grained input signal transmitted by the channel; it solely determines the expectation of channel transmissions given the coarsened input h_i^μ . To ensure dimensional consistency across hidden layers, the output signal of each unit must have the same dimension as its input. Therefore, the correct quantity to consider is the expectation value of the output $j_i = h_i s_i$. This can be obtained by summing over all gate states, or by using the partition function of Eq. (4),

$$\langle j_i \rangle = \langle \hat{h}_i^\mu s_i \rangle_s = \frac{\partial}{\partial \beta_i} \log Z_{i,\mu} = \hat{h}_i^\mu \sigma(\beta_i \hat{h}_i^\mu), \quad (6)$$

that agrees with the definition of the energy flux in statistical mechanics (Bellac et al., 2004). Note that contrary to Eq. (5), the noise parameters β_i cannot be rescaled away. This function was recently obtained in Ref. (Ramachandran et al., 2017) (Swish), through an extensive search algorithm trained with reinforcement learning. In their extensive search, the authors found that activations of the form $a = xf(x)$ better performed on several benchmark datasets. A theoretical study of the performance of Swish from the point of view of information propagation has been proposed in Ref. (Hayou et al., 2018). Our model naturally complements these studies by identifying Swish with the expectation value of the coarse grained input transmitted by each unit. Consider now the limit of a noiseless system $\forall i, \beta_i \rightarrow \infty$:

$$\lim_{\beta_i \rightarrow \infty} \langle j_i \rangle = \hat{h}_i^\mu \theta(\hat{h}_i^\mu) \equiv \max \{ \hat{h}_i^\mu, 0 \} \equiv \text{ReLU}, \quad (7)$$

where $\theta(\cdot)$ is the Heaviside step function and in the last equality we have identified ReLU. To the best of our knowledge, this is the first consistent derivation of ReLU, usually obtained from heuristics. ReLU emerges as the noiseless limit of the mean transmitted information across the units; as such, it is not affected by the dimensional mismatch, see Sec. (2.2). We would like to stress that both Swish and ReLU pass on the expected value of their computation; the latter does it with probability one only if the coarse grained input signal exceeds a threshold, while the former can pass a signal lower than the threshold with a finite probability. A positive signal means that a certain combination of the inputs should be strengthened while a negative one means that it should be weakened, i.e. unlearned; the latter option is absent when using ReLU. In the opposite limit $\beta \ll 1$, Swish becomes linear; therefore, we

can consider linear networks as a noisy limit of non linear ones.

In conclusion, the energy landscape in spin glasses (Mézard et al., 1987; Dominicis & Giardina, 2016) presents an increasing number of degenerate local minima as the temperature/noise is lowered, a feature shared with the Hopfield model of associative memory (Amit & Gutfreund, 1985) and RBM. The effect of noise in FFNs was recently considered in Ref. (Chaudhari et al., 2017),

2.4. On Back-propagation

At the heart of any FFN model is the back propagation algorithm (Hertz et al., 1991; Bishop, 2006). Consider the output layer “L”, then the gradient of the weights is

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}_L} = \frac{1}{m} \sum_{\mu=1}^m \left[\mathbf{e}^\mu \mathbf{g}(\hat{\mathbf{h}}_L^\mu) \right] \mathbf{a}_{L-1} \quad (8)$$

where $\mathbf{e}^\mu \propto y^\mu - \hat{y}^\mu$ is the residual error and $\mathbf{g}(\mathbf{h}_l^\mu) = \boldsymbol{\sigma}(\beta_l \mathbf{h}_l^\mu) [1 + \hat{\mathbf{h}}_l^\mu \beta_l \boldsymbol{\sigma}(-\beta_l \mathbf{h}_l^\mu)]$. In the optimization phase we look for stationary points defined by $\partial \mathcal{L} / \partial \boldsymbol{\theta}_l^\alpha = 0$, where $\boldsymbol{\theta}_l^\alpha = \{\mathbf{w}_l, \mathbf{b}_l, \beta_l\}$. For a linear network, this condition is strictly satisfied if $\mathbf{e}^\mu = 0$. However, in a non linear network we can also have $g(\hat{\mathbf{h}}^\mu) = 0$. In principle, there may be situations in which \mathbf{e}^μ is far from zero but $g(\hat{\mathbf{h}}^\mu) \simeq 0$, in which case learning will not be effective. For a σ activation, $\mathbf{g}(\mathbf{h}_l^\mu) = \boldsymbol{\sigma}(\beta_l \mathbf{h}_l^\mu) \boldsymbol{\sigma}(-\beta_l \mathbf{h}_l^\mu)$, commonly known in physics as a phase space factor (Di-Castro & Raimondi, 2003), describing the transition probability from an occupied to an empty state. Ref. (Tishby & Zaslavsky, 2015; Schwartz-Ziv & Tishby, 2017) show that there are two distinct phases of learning: empirical error minimization (the residual) and representation learning. We can identify the latter with the task of optimizing $g(\hat{\mathbf{h}}^\mu)$. When $\hat{h}_i \gg 1/\beta_i$, i.e. when the signal greatly exceeds the noise, then $\sigma(\beta_i \hat{h}_i) \equiv P(s_i = 1 | \bar{x}_i) \simeq 1$ (\bar{x}_i is the unit’s input) and the back propagated signal is small, being proportional to $g(\hat{h}) \simeq 0$. We then have the paradoxical situation in which, although the lower dimensional representation of the information is considered to be relevant, learning is likely to be inefficient.

Consider now the same limiting behaviour for Swish. If $\hat{h}_i \gg 1/\beta_i$ we now have $g(\hat{h}_i^\mu) \simeq 1$, i.e. the representation learning phase is completed and learning moves towards minimising the empirical error. In the opposite limit, the signal is much smaller than the noise and learning is impossible, as expected. Finally, in the noiseless case one obtains the ReLU solution $g(\hat{h}_i^\mu) = (1, 0)$, for \hat{h}_i respectively greater or smaller than zero. This corresponds to a purely “excitatory”

network, in which representation unlearning is not possible. In other words, the fact that Swish can be negative for $\sigma(\hat{h})/\beta < \hat{h} < 0$ allows for greater flexibility and the possibility to avoid plateaus surrounding local minima and saddle-points. In Ref. (Dauphin et al., 2014), it was proposed that plateaus of zero (or small) curvatures in the loss are mostly responsible for slowing down or preventing convergence of gradient descent. The following section provides a numerical analysis to support this picture.

3. Numerical Analysis

A thorough performance analysis of Swish versus other popular choices of activations was carried out in Ref. (Ramachandran et al., 2017), where it was shown that the former outperformed all other choices on image classification tasks using a convolutional structure. Hereafter, we considered both artificial and experimental datasets trained with ADAM gradient descent (Kingma & Ba, 2015). Given that both datasets lead to the same qualitative features, our analysis is focused on the former and discuss the latter, together with additional details in the (A).

In Fig. (??)(a) we show the loss functions for two binary classification tasks: a linear and a non-linear one, each trained with one and two hidden layers. For the linear task with a single, 10 units layer (adding more units does not improve performance), all three activations attain full train/test accuracy but Swish is the fastest converging. For the non-linear task, ReLU quickly converges to a suboptimal plateau. To obtain a better understanding, we have evaluated two different indices: the fraction of negative eigenvalues of the Hessian $-\alpha$ (Fig. ??(b)) and the fraction of zero eigenvalues $-\gamma$ (Fig. ??(b)). The former measures the ratio of descent to ascent directions on the energy landscape; when α is large, gradient descent can quickly escape a critical point – a saddle point in this case – due to the existence of multiple unstable directions. However, when a critical point exhibits multiple near-zero eigenvalues, roughly captured by γ : in this situation, gradient descent will slowly decrease the training loss. In Ref. (Dauphin et al., 2014) it was noted that energy plateaus are responsible for slowing down or preventing learning. In this case the eigenvalues of the Hessian are zero. Nevertheless, Noether’s theorem infers that these eigenvalues are originated by symmetries of the loss function that somehow prevent lower local minima. In general, we find that for ReLU networks $\gamma \neq 0$, while this is typically not the case for both Swish and sigmoid-networks. Taking the two layer case as a representative example, we show that ReLU networks are

sensitive to fine tuning of the model: choosing a 10 – 2 or a 8 – 5 configuration over the 8 – 2 considered here, greatly improves learning. In stark contrast, Swish networks exhibit consistent performance over a wider choice of architecture/learning parameters. Although the performance impact might be fairly small for small networks, it certainly plays an important role for larger datasets, as discussed in Ref. (Ramachandran et al., 2017). We have also evaluated the fraction of residuals $e^\mu \simeq (\hat{y}^\mu - y^\mu)/m$ closer to zero and found, surprisingly, that Swish greatly outperforms the other activations in minimizing the empirical error, see Fig. (??). In addition, we find that the eigenvalue distribution obtained with ReLU shrinks with increasing training epochs, giving rise to the singular distribution reported in Ref. (Pennington & Bahri, 2017; Sagun et al., 2017). In contrast, Swish show a significantly wider spread in the eigenvalue distribution at the end of training, see sec. (A) for details and discussions, together with results for the MNIST dataset.

Swish training networks can break the symmetries of the loss function and reach extremal points that have higher number of zero residuals (in Physical terms, lower energy minima). This is obtained by preventing large values of the individual components in the Hessian eigenvectors-variables transformation matrices at the minima. In Fig. (??), the Hessian eigenvectors vs the individual variables are plotted in the case of Relu, Sigmoid and Swish networks (see the linear binary classification with two 8-2 hidden layer of 8 and 2 units Fig. (??) bottom left loss function minimization).

4. Conclusions and perspectives

In this work we have introduced an energy-based model that allows systematic construction and analysis of FFNs. It provides a coherent interpretation of the computational process of each and every unit (neuron). It presents a method that overcomes the dimensional mismatch that arises from using heuristic activations. Enforcing dimensional consistency naturally leads to a class of activations with the prime focus of propagating the expectation value of processed signals. Our results provide a theoretical justification of the Swish activation found in Ref. (Ramachandran et al., 2017). We also demonstrate the superiority of the Swish through numerical experiments that reveal the geometry of its loss manifold. We hope this statistical mechanics view can facilitate future studies of FFNs, e.g. to explore the scaling relation between the Swish Hessian’s eigenvalue distributions and the parameters similarly to Ref. (Pennington & Bahri, 2017) for standard activations.

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A. Cross Entropy Loss

In this appendix we present a derivation of the cross entropy loss function using large deviation methods (Mézard & Montanari, 2009). A useful starting point is the definition of the accuracy of a classification task, that is the number of times the network prediction \hat{y} equals the provided solution y . This corresponds to the conditional probability $P(y|\hat{y}) = \mathbb{I}(y = \hat{y})$ in Eq. (??). As \hat{y} is a random variable, we want to know which is the probability of obtaining the true value y in a series of “experiments” in which \hat{y} has a certain probability to be equal to y . According to Eq. (??), and using the standard definition relating the Loss function to the log-probability $\mathcal{L} = -\log P(\mathbf{y})$, we need to evaluate

$$-\log P(\mathbf{y}) = -\log \int d\hat{\mathbf{y}} P(\mathbf{y}|\hat{\mathbf{y}}) P(\hat{\mathbf{y}}), \quad (9)$$

From a physics perspective, the above expression corresponds to an annealed average (Mézard et al., 1987; Dominicis & Giardina, 2016) and we will discuss its meaning at the end of the calculation. For the moment, we assume that we can replace $y \rightarrow y^\mu$ and $\hat{y} \rightarrow \hat{y}^\mu$ directly in Eq. (10), i.e. we fix the random variables on the observed data. Using the Dirac delta as a representation of the Indicator function we have

$$\begin{aligned} P(y) &= \int \left(\prod_\mu d\hat{y}^\mu \right) \prod_\mu \delta(y^\mu - \hat{y}^\mu) P(\hat{y}) \quad (10) \\ &= \int \left(\prod_\mu \frac{d\lambda^\mu}{2\pi} \right) \prod_\mu e^{i \sum_\mu \lambda^\mu y^\mu} \chi(\lambda^\mu). \end{aligned}$$

where we have introduced m Lagrange multipliers λ to enforce the δ -function constraint and identified the

characteristic function

$$\chi(\lambda^\mu) = \int \left(\prod_\mu d\hat{y}^\mu \right) P(\hat{y}^\mu) e^{-i \sum_\mu \lambda^\mu \hat{y}^\mu} \quad (11)$$

Let us consider the case of i.i.d. examples, distributed according to the Bernoulli distribution:

$$P(\hat{y}^\mu) = \int d\boldsymbol{\theta} \{q^\mu(\boldsymbol{\theta}) \delta(\hat{y}^\mu - 1) + (1 - q^\mu(\boldsymbol{\theta})) \delta(\hat{y}^\mu - 0)\}, \quad (12)$$

where each outcome is either 1 or 0 with a sample dependent probability $q^\mu(\boldsymbol{\theta})$ being the output value of a Neural Network solving a binary classification task; as such, q has the functional form of a sigmoid function with $\boldsymbol{\theta}$ a set of network parameters. In this case, Eq. (13) reads

$$\chi(\lambda^\mu) = \int d\boldsymbol{\theta} [q^\mu(\boldsymbol{\theta}) e^{-i \lambda^\mu} + (1 - q^\mu(\boldsymbol{\theta}))]. \quad (13)$$

Using this expression back in Eq. (12) we arrive at the intermediate result

$$\begin{aligned} P(y) &= \int d\boldsymbol{\theta} \int \left(\prod_\mu \frac{d\lambda^\mu}{2\pi} \right) e^{i \sum_\mu \lambda^\mu y^\mu + \sum_\mu \log[q^\mu e^{-i \lambda^\mu} + (1 - q^\mu)]} \\ &= \int \left(\prod_\mu \frac{d\lambda^\mu}{2\pi} \right) e^{m S[\lambda]}. \end{aligned} \quad (14)$$

For a large number of training examples m , we can solve the above integral using the steepest descent, i.e. using a maximum likelihood approach. This fixes the value of the Lagrange multipliers:

$$\begin{aligned} \frac{\partial S[\lambda]}{\partial \lambda^\mu} &= i y^\mu - \frac{i q^\mu e^{-i \lambda^\mu}}{q^\mu e^{-i \lambda^\mu} + (1 - q^\mu)} = 0 \\ &\rightarrow -i \lambda_c^\mu = \log \frac{y^\mu (1 - q^\mu)}{q^\mu (1 - y^\mu)} \end{aligned} \quad (15)$$

Using the optima back in Eq. (14) we arrive after some simple algebra to the expression for the cross-entropy:

$$\begin{aligned} P(y) &\simeq \int d\boldsymbol{\theta} e^{m S[\lambda_c, \boldsymbol{\theta}]} \quad (16) \\ S[\lambda_c] &= \frac{1}{m} \sum_\mu \{y^\mu \log[q^\mu(\boldsymbol{\theta})] + (1 - y^\mu) \log[1 - q^\mu(\boldsymbol{\theta})]\}, \end{aligned}$$

up to an additive constant depending only on y . The final step consists in evaluating the $\boldsymbol{\theta}$ integral again for $m \gg 1$, and take the maximum likelihood value $\boldsymbol{\theta}^*$.

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