Learning Neuron Non-Linearities with Kernel-Based Deep Neural Networks

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Abstract

The effectiveness of deep neural architectures has been widely supported in terms of both experimental and foundational principles. There is also clear evidence that the activation function (e.g. the rectifier and the LSTM units) plays a crucial role in the complexity of learning. Based on this remark, this paper discusses an optimal selection of the neuron non-linearity in a functional framework that is inspired from classic regularization arguments. It is shown that the best activation function is represented by a kernel expansion in the training set, that can be effectively approximated over an opportune set of points modeling 1-D clusters. The idea can be naturally extended to recurrent networks, where the expressiveness of kernel-based activation functions turns out to be a crucial ingredient to capture long-term dependencies. We give experimental evidence of this property by a set of challenging experiments, where we compare the results with neural architectures based on state of the art LSTM cells.

1 Introduction

By and large, the appropriate selection of the activation function in deep architectures is regarded as an important choice for achieving challenging performance. For example, the rectifier function \cite{7} has been playing an important role in the impressive scaling up of nowadays deep nets. Likewise, LSTM cells \cite{8} are widely recognized as the most important ingredient to face long-term dependencies when learning by recurrent neural networks. Both choices come from insightful ideas on the actual non-linear process taking place in deep nets. At a first glance, one might wonder why such an optimal choice must be restricted to a single unit instead of extending it to the overall function to be learned. In addition, this general problem has been already been solved; its solution \cite{12, 5, 6} is in fact at
the basis of kernel machines, whose limitations as shallow nets, have been widely addressed (see e.g. [10, 11]). However, the optimal formulation given for the neuron non-linearity enjoys the tremendous advantage of acting on 1-D spaces. This strongly motivates the reformulation of the problem of learning in deep neural network as a one where the weights and the activation functions are jointly determined by optimization in the framework of regularization operators [13], that are used to enforce the smoothness of the solution. The idea of learning the activation function is not entirely new. In [15], activation functions are chosen from a pre-defined set and combine this strategy with a single scaling parameter that is learned during training. It has been argued that one can think of this function as a neural network itself, so as the overall architecture is still characterized by a directed acyclic graph [3]. Other approaches learn activation functions as piecewise linear [1], doubled truncated gaussian [14] or Furier series [4]. In this paper, it is proven that, like for kernel machines, the optimal solution can be expressed by a kernel expansion, so as the overall optimization is reduced to the discovery of a finite set of parameters. The risk function to be minimized contains the weights of the network connections, as well as the parameters associated with the the points of the kernel expansion. Hence, the classic learning of the weights of the network takes place with the concurrent development of the optimal shape of the activation functions, one for each neuron. As a consequence, the machine architecture turns out to enjoy the strong representational issues of deep networks in high dimensional spaces that is conjugated with the elegant and effective setting of kernel machines for the learning of the activation functions. The powerful unified regularization framework is not the only feature that emerges from the proposed architecture. Interestingly, unlike most of the activation functions used in deep networks, those that are typically developed during learning, are not necessarily monotonic. This property has a crucial impact in their adoption in classic recurrent networks, since this properly addresses classic issues of gradient vanishing when capturing long-term dependencies. Throughout this paper, recurrent networks with activation functions based on kernel expansion, are referred to as Kernel-Based Recurrent Networks (KBRN). The intuition is that the associated iterated map can either be contractive or expansive. Hence, while in some states the contraction yields gradient vanishing, in others the expansion results in to gradient pumping, which allows the neural network to propagate information back also in case of long time dependences. The possibility of implementing contractive and expanding maps during the processing of a given sequence comes from the capabilities of KBRN to develop different activation functions for different neurons that are not necessarily monotonic. This variety of units is somewhat related to the clever solution proposed in LSTM cells [8], where the authors early realized that there was room for getting rid of the inherent limitation of the contractive maps deriving from sigmoidal units. The given experimental results provide evidence of this property on challenging benchmarks that are inspired to seminal paper [2], where the distinctive information for classification of long sequences is only located in the first positions, while the rest contains uniformly distributed noisy information. We get very promising results on these benchmarks when
without loss of generality we will also assume that:

which accumulates the empirical risk and a regularization term based regular-

The learning problem can then be formulated as a double optimization problem

with

a specific function

Instead of

The learning process is based on the training set T_N = \{ (e^\kappa, y^\kappa) \in \mathbb{R}^{I_f} \times \mathbb{R}^{O} | \kappa = 1, \ldots, N \}. Given an input vector z = (z_1, z_2, \ldots, z_H), the output associated with the vertices of the graph is computed as follows:

\[ x_i(z) = z_i[i \in I] + f_i(a_i)[i \notin I], \]

with \( a_i = \sum_{j \in \text{pa}(i)} w_{ij} x_j + b_i \), where \( \text{pa}(i) \) are the parents of neuron \( i \), and \( f_i: \Omega_\Lambda \rightarrow \mathbb{R} \) are one dimensional real functions; \( \Omega_\Lambda := [-\Lambda, \Lambda] \), with \( \Lambda \) chosen big enough, so that Eq. (1) is always well defined. Now let \( f = (f_1, f_2, \ldots, f_n) \) and define the output function of the network \( F(.,w,b;f): \mathbb{R}^{I_f} \rightarrow \mathbb{R}^{O} \) by

\[ F_i(z,w,b;f) := x_{i+|I|+H}(z), \quad i = 1, \ldots, |O|. \]

The learning problem can then be formulated as a double optimization problem defined on both the weights \( w, b \) and on the activation functions \( f_i \). It is worth mentioning that while the optimization on the weights of the graph reflects all important issues connected with the powerful representational properties of deep nets, the optimal discovery of the activation functions are somewhat related to the framework of kernel machines. Such an optimization is defined with respect to the following objective function:

\[ E(f;w,b) := \frac{1}{2} \sum_{i=1}^{n} (P f_i, P f_i) + \sum_{\kappa=1}^{N} V(e^\kappa, y^\kappa, F(e^\kappa, w, b; f)), \]

which accumulates the empirical risk and a regularization term based regularization operators [13]. Here, we indicate with \( (\cdot, \cdot) \) the standard inner product of \( L^2(\Omega_\Lambda) \), with \( P \) a differential operator of degree \( p \), while \( V \) is a suitable loss function.

Clearly, one can optimize \( E \) by independently checking the stationarity with respect to the weights associated with the neural connections and the stationarity

\[ \text{We are using here the Iverson’s notation: Given a statement } A, \text{ we set } [A] \text{ to 1 if } A \text{ is true and to 0 if } A \text{ is false.} \]
with respect to the activation functions. Now we show that the stationarity condition of $E$ with respect to the functional variables $f$ (chosen in a functional space $X_p$ that depends on the order of differential operator $P$) yields a solution that is very related to classic case of kernel machines that is addressed in [13]. If we consider a variation $v_i \in C^\infty_c(\Omega \Lambda)$ with vanishing derivatives on the boundary $\partial \Omega \Lambda$ up to order $p - 1$ and define $\varphi_i(t) := E(f_1, \ldots, f_i + tv_i, \ldots, f_n; w, b)$. The first variation of the functional $E$ along $v_i$ is therefore $\varphi_i'(0)$. When using arguments already discussed in related papers [12, 5, 13] we can easily see that

$$\varphi_i'(0) = \int_{\Omega \Lambda} \left( Lf_i(a) + \sum_{\kappa=1}^N \alpha_{i\kappa} \delta a_{i\kappa}(a) \right) v_i(a) \, da,$$

where $\alpha_{i\kappa} = \nabla_k V \cdot \partial f_i F$ and $L = P^* P$, $P^*$ being the adjoint operator of $P$. We notice in passing that the functional dependence of $E$ on $f$ is quite involved, since it depends on the compositions of liner combinations of the functions $f_i$ (see Figure 1(a)). Hence, the given expression of the coefficients $\alpha_{i\kappa}$ is a rather a formal equation that, however, dictates the structure of the solution.

The stationarity conditions $\varphi_i'(0) = 0$ reduce to the following Euler-Lagrange (E-L) equations

$$L f_i(a) + \sum_{\kappa=1}^N \alpha_{i\kappa} \delta a_{i\kappa}(a) = 0, \quad i = 1 \ldots n,$$

where $a_{i\kappa}$ is the value of the activation function on the $\kappa$-th example of the training set. Let $g$ be the Green function of the operator $L$, and let be $k$ the

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Footnote: Here, we are assuming here that the values of the functions in $X_p$ at the boundaries together with the derivatives up to order $p - 1$ are fixed.
solution of $L k = 0$. Then, we can promptly see that

$$f_i(a) = k(a) - \sum_{\kappa=1}^{N} \alpha_{\kappa}^i g(a - a_{\kappa}^i)$$

(4)

is the general form of the solution of Eq. (3). Whenever $L$ has null kernel, then this solution is reduced to an expansion of the Green function over the points of the training set. For example, this happens in the case of the pseudo differential operator that originates the Gaussian as the Green function. If we choose $P = d/dx$, then $L = -d^2/dx^2$. Interestingly, the Green function of the second derivative is the rectifier $g(x) = -\frac{1}{2}(|x| + x)$ and, moreover, we have $k(x) = mx + q$. In this case

$$f_i(a) = \theta_i a + \nu_i + \frac{1}{2} \sum_{\kappa=1}^{N} \alpha_{\kappa}^i |a - a_{\kappa}^i|,$$

(5)

where $\theta_i = m + \frac{1}{2} \sum_{\kappa=1}^{N} \alpha_{\kappa}^i$, while $\nu_i = q - \frac{1}{2} \sum_{\kappa=1}^{N} \alpha_{\kappa}^i a_{\kappa}^i$. Because of the representation structure expressed by Eq. (4), the objective function the original optimization problem collapses to a standard finite-dimensional optimization on

$$\hat{E}(\alpha, w, b) := E\left(k(a) - \sum_{\kappa} \alpha_{\kappa}^i g(a - a_{\kappa}^i); w, b \right) = R(\alpha) + \sum_{\kappa=1}^{N} V(e^\kappa, y^\kappa, \hat{F}(e^\kappa, w, b; \alpha));$$

here $R(\alpha)$ is the regularization term and $\hat{F}(e^\kappa, w, b; \alpha) := F(e^\kappa, w, b; k(a) - \sum_{\kappa} \alpha_{\kappa}^i g(a - a_{\kappa}^i))$. This collapse of dimensionality is the same which leads to the dramatic simplification that gives rise to the theory of kernel machines. Basically, in all cases in which the Green function can be interpreted as a kernel, this analysis suggests the neural architecture depicted in Figure 1, where we can see the integration of graphical structures, typical of deep nets, with the representation in the dual space that typical of kernel methods.

We can promptly see that the idea behind kernel-based deep networks can be extended to cyclic graphs, that is to recurrent neural networks. In that case, the analogous of Eq. (1) is:

$$h_{t+1}^i = f_i(a_{t+1}^i); \quad a_{t+1}^i = b_i + \sum_{j \in p_a_{t+1}(i)} w_{ij} h_j^t + \sum_{j \in p_{a_{t+1}}(i)} u_{ij} x_{j}^{t+1}.$$  

Here we denote with $x_{j}^t$ the input at step $t$ and with $h_{j}^t$ the state of the network. The set $p_{a_{t+1}}(i)$ contains the vertices $j$ that are parents of neuron $i$; the corresponding arcs $(j, i)$ are associated with a delay, while $p_a(i)$ vertices $j$ with non-delayed arcs $(j, i)$. The extension of learning in KBDNN to the case of recurrent nets is a straightforward consequence of classic Backpropagation Through Time.

\footnote{Here we omit the dependencies of the optimization function from the parameters that defines $k$.}
3 Approximation and algorithmic issues

The actual experimentation of the model described in the previous section requires to deal with a number of important algorithmic issues. In particular, we need to address the typical problem associated with the kernel expansion over the entire training set, that is very expensive in computational terms. However, we can early realize that KBDNNs only require to express kernel in 1-D, which dramatically simplify the kernel approximation. Hence, instead of expanding $f_i$ over the entire training set, we can use a number of points $d$ with $d \ll N$. This means that the expansion in Eq. (4) is approximated as follows

$$f_i(a) \approx k(a) - \sum_{k=1}^{d} \chi^k_i g(a - c^k_i),$$

where $c^k_i$ and $\chi^k_i$ are the centers and parameters of the expansion, respectively. Notice that $\chi^k_i$ are replacing $\alpha^k_i$ in the formulation given in Section 2. We consider $c^k_i$ and $\chi^k_i$ as parameters to be learned, and integrate them in the whole optimization scheme.

In the experiments described below we use the rectifier (ReLU) as Green function ($g(x) = -\frac{1}{2}(|x| + x)$) and neglect the linear terms from both $g(x)$ and $k(x)$. We can easily see that this is compatible with typical requirements in machine learning experiments, where in many cases the expected solution is not meaningful with very large inputs. For instance, the same assumption is typically at the basis of kernel machines, where the asymptotic behavior is not typically important. The regularization term $R(\chi)$ can be inherited from the regularization operator $P$. For the experiments carried out in this paper we decided to choose the $\ell_1$ norm:

$$R(\chi) \approx \lambda_\chi \sum_{1 \leq k \leq d} |\chi^k_i|,$$

with $\lambda_\chi \in \mathbb{R}$ being an hyper-parameter that measures the strength of the regularization.

In a deep architecture, when stacking multiple layers of kernel-based units, the non-monotonicity of the activation functions implies the absence of guarantees about the interval on which these functions operate, thus requiring them to be responsive to very heterogeneous inputs. In order to face this problem and to allow kernel-based units to concentrate their representational power on limited input ranges, it is possible to apply a normalization [9] to the input of the function. In particular, given $f_i(a^k_i)$, $a^k_i$ can be normalized as:

$$\hat{a}^k_i = \gamma_i \left(\frac{a^k_i - \mu_i}{\sigma_i}\right) + \beta_i; \quad \text{where} \quad \mu_i = \frac{1}{N} \sum_{k=1}^{N} a^k_i; \quad \sigma_i = \frac{1}{N} \sum_{k=1}^{N} (a^k_i - \mu_i)^2;$$

while $\gamma_i$ and $\beta_i$ are additional trainable parameters.

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4This choice is due to the fact that we want to enforce the sparseness of $\chi$, i.e. to use the smallest number of terms in expansion 6.
Figure 2: **XOR.** The plots show the activation functions learned by the simplest KBDN which consists of one unit only for the 2-dim (2a) and 4-dim (2b) XOR. The first/second row refer to experiments with without/with regularization, whereas the three columns correspond with the chosen number of point for the expansion of the Green function $d = 50, 100, 300$.

Figure 3: **Charging Problem.** The plot shows the accuracy obtained a by recurrent nets which classic sigmoidal unit, LSTM cell, and KB unit. The horizontal axis is in logarithmic scale.

4 Experiments

We carried out several experiments in different learning settings to investigate the effectiveness of the KBDNN with emphasis on the adoption of kernel-based units in recurrent networks for capturing long-term dependences. Clearly, KBDNN architectures require to choose both the graph and the activation function. As it will be clear in the reminder of this section, the interplay of these choices leads to gain remarkable properties.

**The XOR problem.** We begin presenting a typical experimental set up in the classic XOR benchmark. In this experiment we chose a single unit with the Green function $g(z) = |z|$, so as $y = f(w_1 z_1 + w_2 z_2 + b)$ turns out to be

$$y = \sum_{k=1}^{d} \chi^{k} |w_1 z_1 + w_2 z_2 + b - c^k|$$

where $w_1, w_2$ and $b$ are trainable variables and the learning of $f$ corresponds
with the discovery of both the centroids $c^k$ and the associated weights $\chi^k$. The simplicity of this learning task allows us to underline some interesting properties of KBDNNs. We carried out experiment by selecting a number of points for the expansion of the Green function that ranges from 50 to 300. This was done purposely to assess the regularization capabilities of the model, that is very much related to what typically happens with kernel machines. In Figure 2, we can see the neuron function $f$ at the end of the learning process under different settings. In the different columns, we plot function $f$ with a different numbers $d$ of clusters, while the two rows refer to experiments carried out with and without regularization. As one could expect, the learned activation functions become more and more complex as the number of clusters increases. However, when performing regularization, the effect of the kernel-based component of the architecture plays a crucial role by smoothing the functions significantly.

The charging problem. Let us consider a dynamical system which generates a Boolean sequence according to the model

$$
\begin{align*}
  h_t &= x_t + [h_{t-1} - 1 > 0] \cdot (h_{t-1} - 1) \\
  y_t &= [h_t > 0],
\end{align*}
$$

(7)

where $h_{t-1} = 0$, $x = (x_t)$ is a sequence of integers and $y = (y_t)$ is a Boolean sequence, that is $y_t \in \{0, 1\}$. An example of sequences generated by this system is the following:

$t = 0 1 2 3 4 5 6 7 8 9 10 \ldots$

$x_t = 0 0 0 4 0 0 0 0 0 0 0 \ldots$

$y_t = 0 0 0 1 1 1 1 0 0 0 0 \ldots$

Notice that the system keeps memory when other 1 bit are coming, that is

$t = 0 1 2 3 4 5 6 7 8 9 10 \ldots$

$x_t = 0 0 0 4 0 2 0 0 0 0 0 \ldots$

$y_t = 0 0 0 1 1 1 1 1 1 0 0 \ldots$

The purpose of this experiment was that of checking what are the learning capabilities of KBRN to approximate sequences generated according to Eq. 7. The intuition is that a single KB-neuron is capable to charge the state according to an input, and then to discharge it until the state is reset. We generated sequences $\langle x_t \rangle$ of length $L = 30$. Three random element of each sequence were set with a random number ranging from 0 to 9. We compared KBRN, RNN with sigmoidal units, and recurrent with LSTM cells, with a single hidden unit. We used a KBRN unit with $d = 20$ centers to approximate the activation function. The algorithm used for optimization used the Adam algorithm with $\lambda = 0.001$ in all cases. Each model was trained for 10000 iterations with mini-batches of size 500. Figure 3 shows the accuracy on a randomly generated test set of size 25000 during the training process. The horizontal axis is in logarithmic scale. The horizontal axis is in logarithmic scale.

Learning Long-Term dependencies. We carried out a number of experiments aimed at investigating the capabilities of KBRN in learning tasks where
we need to capture long-term dependencies. The difficulties of solving similar problems were addressed in [2] by discussions on gradient vanishing that is mostly due to the monotonicity of the activation functions. The authors also provided very effective yet simple benchmarks to claim that classic recurrent networks are unable to classify sequences where the distinguishing information is located only at the very beginning of the sequence; the rest of the sequence was supposed to be randomly generated. We defined a number of benchmarks inspired by the one given in [2], where the decision on the classification of sequence \( \langle x_t \rangle \) is contained in the first \( L \) bits of a Boolean sequence of length \( T \gg L \). We compared KBRN and recurrent nets with LSTM cells using an architecture where both networks were based on 20 hidden units. We used the Adam algorithm with \( \lambda = 0.001 \) in all cases. Each model was trained for a maximum of 100,000 iterations with mini-batches of size 500; for each iteration, a single weight update was performed. For the LSTM cells, we used the standard implementation provided by TensorFlow (following [16]). For KBRN we used a number of centroids \( d = 100 \) and the described normalization.

We generated automatically a set of benchmarks with \( L = 2 \) and variable length \( T \), where the binary sequences \( \langle x_t \rangle \) can be distinguished when looking simply at the first two bits, while the the rest is a noisy string with uniformly random distribution. Here we report some of our experiments when choosing the first two discriminant bits according to the \( \lor, \land, \oplus \) and \( \equiv \) functions.

For each Boolean function, that was supposed to be learned, and for several sequence lengths (up to 50), we performed 5 different runs, with different initialization seeds. A trial was considered successful if the model was capable of learning the function before the maximum allowed number of iterations was reached.
Figure 5: Capturing Long-Term dependencies. Number of successful trials and average number of iterations for a classification problem when the $\lor$, $\land$, $\oplus$ and $\equiv$ functions are used to determine the target, given the first two discriminant bits.
reached. In Figure 5 we present the results of these experiments. Each of the four quadrants of Figure 5 is relative to a different Boolean function, and reports two different plots. The first one has the sequence length on the $x$-axis and the number of successful trials on the $y$-axis. The second plot has the sequence length on the $x$-axis and, on the $y$-axis, the average number of iterations required to solve the task. The analysis of these plots allows us to draw a couple of interesting conclusions: (i) KBRN architectures are capable of solving the problems in almost all cases, regardless of the sequence length, while recurrent networks with LSTM cells started to experiment difficulties for sequences longer than 30, and (ii), whenever convergence is achieved, KBRN architectures converge significantly faster than LSTM. In order to investigate with more details the capabilities of KBRN of handling very long sequences, we carried out another experiment, that was based on the benchmark that KBRN solved with more difficulty, namely the equivalence ($\equiv$) problem. We carried out a processing over sequences with length 60, 80, 100, 150, and 200. In Figure 6 we report the results of this experiment. As we can see, KBRN are capable of solving the task even with sequences of length 150, eventually failing with sequences of length 200.

5 Conclusions

In this paper we have introduced Kernel-Based Deep Neural Networks. The proposed KBDNN model is characterized by the classic primal representation of deep nets, that is enriched with the expressiveness of activation functions given by kernel expansion. The idea of learning the activation function is not entirely new. However, in this paper we have shown that the KBDNN representation turns out to be the solution of a general optimization problem, in which both the weights, that belong to a finite-dimensional space, and the activation function, that are chosen from a functional space are jointly determined. This bridges
naturally the powerful representation capabilities of deep nets with the elegant
and effective setting of kernel machines for the learning of the neuron functions.

A massive experimentation of KBDNN is still required to assess the actual
impact of the appropriate activation function in real-world problems. However,
this paper already proposes a first important conclusion which involves recurrent
networks, that are based on this kind of activation function. In particular, we
have provided both theoretical and experimental evidence to claim that the
KBRN architecture exhibits an ideal computational structure to deal with classic
problems of capturing long-term dependencies.

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