Training of Deep Neural Networks based on Distance Measures using RMSProp

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Abstract—The vanishing gradient problem was a major obstacle for the success of deep learning. In recent years it was gradually alleviated through multiple different techniques. However the problem was not really overcome in a fundamental way, since it is inherent to neural networks with activation functions based on dot products. In a series of papers, we are going to analyze alternative neural network structures which are not based on dot products. In this first paper, we revisit neural networks built up of layers based on distance measures and Gaussian activation functions. These kinds of networks were only sparsely used in the past since they are hard to train when using plain stochastic gradient descent methods. We show that by using Root Mean Square Propagation (RMSProp) it is possible to efficiently learn multi-layer neural networks. Furthermore we show that when appropriately initialized these kinds of neural networks suffer much less from the vanishing and exploding gradient problem than traditional neural networks even for deep networks.

Index Terms—deep neural networks, vanishing problem, neural networks based on distance measures

1 INTRODUCTION

Most types of neural networks nowadays are trained using stochastic gradient descent (SGD). However gradient-based approaches (batched and stochastic) suffer from several drawbacks. The most critical drawback is the vanishing gradient problem, which makes it hard to learn the parameters of the "front" layers in an \( n \)-layer network. This problem becomes worse as the number \( n \) of layers in the architecture increases. This is especially critical in recurrent neural networks [10], which are trained by unfolding them into very deep feedforward networks. For each time step of an input sequence processed by the network a new layer is created. The second drawback of gradient-based approaches is the potential to get stuck at local minima and saddle points.

To overcome the vanishing gradient problem, several methods were proposed in the past [5][7][9][10]. Early methods consisted of the pre-training of the weights using unsupervised learning techniques in order to establish a better initial configuration, followed by a supervised fine-tuning through backpropagation. The unsupervised pre-training was used to learn generally useful feature detectors. At first, Hinton et. al. used stacked Restricted Boltzmann Machines (RBM) to do a greedy layer-wise unsupervised training of deep neural networks [9].

The Xavier Initialization [5] by Glorot et. al. (after Glorot’s first name) was a further step to overcome the vanishing gradient problem. In Xavier initialization the initial weights of the neural networks are sampled from a Gaussian distribution where the variance is a function of the number of neurons in a given layer. At about the same time Rectified Linear Units (ReLU) where introduced, a non-linearity that is scale-invariant around 0 and does not saturate at large input values [7]. Both Xavier Initialization and ReLUs alleviated the problems the sigmoid activation functions had with vanishing gradient.

Another method particularly used to cope with the vanishing gradient problem for recurrent neural networks is the Long Short-Term Memory (LSTM) network [10]. By introducing memory cells the gradient can be propagated back to a much earlier time without vanishing.

One of the newest and most effective ways to resolve the vanishing gradient problem is with residual neural networks (ResNets) [8]. ResNets yield lower training error (and test error) than their shallower counterparts simply by reintroducing outputs from shallower layers in the network to compensate for the vanishing data.

The main reason behind vanishing gradient problem is the fundamental difference between the forward and the backward pass in neural networks with activation functions based on dot products [1]. While the forward pass is highly non-linear in nature, the backward pass is completely linear due to the fixed values of the activations obtained in the forward pass. During the backpropagation the network behaves as a linear system and suffers from the problem of linear systems, which is the tendency to either explode or die when iterated.

In this paper, we address the problem of vanishing gradient by exploring the properties of neural networks based on distance measures which are an alternative to neural networks based on dot products [3]. In neural networks based on distance measures the weight vectors of neurons represent landmarks in the input space. The activation of a neuron is computed from the weighted distance of the the input vector from the corresponding landmark. Determining the distance is possible by applying different measures. In this work, we apply the most commonly used Gaussian kernel [3]. The parameters of the network to be learnt consist of both the landmarks and the weights of the distance measure.

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2 Basic Principle

In this section, we show how a network of Gaussian layers interconnected in a feed-forward way can be used to approximate arbitrary bounded continuous functions. For demonstration purposes, we use a simple 1D example, see Fig. 1.

\[ x^{(1)}(\theta) = \exp\left(-\frac{1}{2} \cdot \left[r_{x}^{(0)}\right]^{2} \cdot (\theta - c_{x}^{(0)})^{2}\right), \quad (1) \]

and

\[ y^{(1)}(\theta) = \exp\left(-\frac{1}{2} \cdot \left[r_{y}^{(0)}\right]^{2} \cdot (\theta - c_{y}^{(0)})^{2}\right), \quad (2) \]

with \( r_{x}^{(0)}, c_{x}^{(0)}, r_{y}^{(0)}, c_{y}^{(0)} \in \mathbb{R} \). The shapes of (1) and (2) as functions of \( \theta \) are depicted in Fig. 2.

The two outputs of the first layer can be interpreted as the x-coordinate and the y-coordinate of a 2D trajectory. The resulting trajectory is depicted in Fig. 3.

\[ f(\theta) = \frac{1}{2} + \frac{1}{6} \left(\frac{\sin(3\pi \theta - \pi/4)}{\exp(2/5 \cdot \theta)} + \frac{\cos(5\pi \theta - \pi/3)}{\exp(-4/5 \cdot \theta)}\right) \quad (4) \]

The shape of (4) together with its approximation is depicted in Fig. 6. The parameters of the network are optimized using the backpropagation algorithm introduced in the next section. The (Root Mean Square) RMS of the approximation is 0.008.
The described method can be extended to an arbitrary number of input and output dimensions.

3 Forward Pass

Layer \( l \) has \( s_i \) inputs denoted by \( a_i^{(l)} \) and \( s_{l+1} \) outputs denoted by \( a_j^{(l+1)} \), as depicted in Fig. 7. The value of \( j \)-th output depends on all \( s_i \) inputs of layer \( l \) and is calculated using the following Gaussian function:

\[
a_j^{(l+1)} = \exp \left( -\frac{1}{2} \sum_{i=1}^{s_i} \left[ r_j^{(l)} \right]_i \cdot (a_i^{(l)} - [c_j^{(l)}]_i)^2 \right),
\]

where \( j \in \{1, \ldots, s_{l+1}\} \). The terms \( r_j^{(l)} \) and \( c_j^{(l)} \) denote the \( i \)-th element of vector \( r_j^{(l)} \in \mathbb{R}^{s_l} \) and \( c_j^{(l)} \in \mathbb{R}^{s_l} \) respectively.

![Fig. 7. Architecture of layer \( l \) and corresponding parameters](image)

4 Cost Function

A cost function measures how well the neural network performs to map training samples \( x^{(i)} \) to the desired output \( y^{(i)} \). We denote the cost function with respect to a single training sample to be:

\[
J(R, C; x^{(i)}, y^{(i)})
\]

where \( R \) and \( C \) represent the parameters of the network based on distance measures. Given a training set of \( m \) samples, the overall cost function is an average over the cost functions (6) for individual training examples plus a regularization term [6]. All cost functions typically used in practice with neural networks with activation functions based on dot products can be applied as well.

The activations of the output layer are \( a_j^{(L+1)}, j \in \{1, \ldots, s_{L+1}\} \), where \( L \) denotes the number of layers in the network, see Fig. 8. The output activations depend on both the input \( x^{(i)} \) and the parameters \( R \) and \( C \) of the network: \( a_j^{(L+1)}(R, C; x^{(i)}) \), which is implicitly assumed in following formulas.

![Fig. 8. Input and output activation functions of a network with \( L \) layers](image)

In particular for regression tasks we are using the quadratic cost:

\[
J(R, C; x^{(i)}, y^{(i)}) = \sum_{j=1}^{s_{L+1}} (a_j^{(L+1)} - y_j^{(i)})^2,
\]

where \( x^{(i)} \in \mathbb{R}^{s_l} \) is the input vector and \( y_j^{(i)} \in \mathbb{R}^{s_{L+1}} \) is the continuous target value. For classification purposes, we use a Softmax output layer and the cross-entropy function [2]:

\[
J(R, C; x^{(i)}, y^{(i)}) = \sum_{j=1}^{s_{L+1}} y_j^{(i)} \log \left( \frac{\exp a_j^{(L+1)}}{\sum_{k=1}^{s_{L+1}} \exp a_k^{(L+1)}} \right),
\]

where \( y_j^{(i)} \) is a one-hot encoded target output vector. In case a Softmax output layer is used, the Gaussian activation function in last layer is omitted:

\[
a_j^{(L+1)} = \frac{1}{2} \sum_{i=1}^{s_i} \left[ r_j^{(L)} \right]_i \cdot (a_i^{(L)} - [c_j^{(L)}]_i)^2,
\]

5 Backward Pass

As in conventional neural networks backpropagation is easily adaptable [12][13]. Let us denote the partial derivative of the cost function w.r.t the activation function of layer \( l+1 \) as \( \delta_j^{(l+1)} = \partial J/\partial a_j^{(l+1)} \).

The upper partial derivative of the preceding layer is backpropagated using the following formula:

\[
\delta_i^{(l)} = -\sum_{j=1}^{s_{l+1}} \delta_j^{(l+1)} \cdot a_j^{(l+1)} \cdot \left[ r_j^{(l)} \right]_i \cdot (a_i^{(l)} - [c_j^{(L)}]_i),
\]

where \( i \in \{1, \ldots, s_l\} \). The update of the centroid parameters in layer \( l \) is calculated via:

\[
\frac{\partial J}{\partial [c_j^{(l)}]_i} = \delta_j^{(l+1)} \cdot a_j^{(l+1)} \cdot \left[ r_j^{(l)} \right]_i \cdot (a_i^{(l)} - [c_j^{(l)}]_i),
\]

where \( j \in \{1, \ldots, s_{l+1}\} \) and \( i \in \{1, \ldots, s_i\} \). The update of the radius parameters in layer \( l \) is:

\[
\frac{\partial J}{\partial [r_j^{(l)}]_i} = -\delta_j^{(l+1)} \cdot a_j^{(l+1)} \cdot \left[ r_j^{(l)} \right]_i \cdot (a_i^{(l)} - [c_j^{(l)}]_i).
\]
6 RMSProp

It is not possible to train the neural networks based on distance measures and Gaussian activations functions using only plain mini-batch gradient descent or momentum. No or only extremely slow convergence can be achieved that way. This is the case even for shallow networks. The solution is to apply RMSProp (Root Mean Square Propagation), which renders the training possible in the first place [14].

In RMSProp, the learning rate is adapted for each of the parameter vectors \( c_j^{(l)} \) and \( r_j^{(l)} \), \( \forall j \in \{1, \ldots, s_l\} \) and \( \forall l \in \{1, \ldots, L\} \). The idea is to keep a moving average of the squared gradients over adjacent mini-batches for each weight:

\[
\bar{v} \left( c_j^{(l)}, t \right) = \gamma \bar{v} \left( c_j^{(l)}, t - 1 \right) + \left( 1 - \gamma \right) \left( \partial J / \partial c_j^{(l)} \right)^2
\]

\[
\bar{v} \left( r_j^{(l)}, t \right) = \gamma \bar{v} \left( r_j^{(l)}, t - 1 \right) + \left( 1 - \gamma \right) \left( \partial J / \partial r_j^{(l)} \right)^2
\]

where \( \gamma \) is the forgetting factor, typically 0.9. Next the learning rate for a weight is divided by that moving average:

\[
c_j^{(l)} := c_j^{(l)} - \frac{\eta}{\sqrt{\bar{v} \left( c_j^{(l)}, t \right)}} \cdot \frac{\partial J / \partial c_j^{(l)}}{\sqrt{\bar{v} \left( c_j^{(l)}, t \right)}}
\]

\[
r_j^{(l)} := r_j^{(l)} - \frac{\eta}{\sqrt{\bar{v} \left( r_j^{(l)}, t \right)}} \cdot \frac{\partial J / \partial r_j^{(l)}}{\sqrt{\bar{v} \left( r_j^{(l)}, t \right)}}
\]

RMSProp has shown excellent adaptation of learning rate in different applications.

7 Initialization

As in neural networks based on dot products [5], a sensible initialization of the weights is crucial for convergence, especially when training deep neural networks. The initialization of the weights controlling the center of the Gaussian functions is straightforward:

\[
\left[ c_j^{(l)} \right]_i \in \mathcal{N} \left( \mu_c, \sigma_c^2 \right),
\]

where \( \mathcal{N} \) denotes a normal distribution. Experiments show that values \( \mu_c = 0.63 \) and \( \sigma_c = 0.1 \) work well for most network architectures. The initialization in (15) does not depend neither on the number of inputs nor on the number of outputs of a layer.

The initialization of the weights controlling the radii of the Gaussian functions is slightly more complicated:

\[
r_j^{(l)} \in \mathcal{N} \left( \mu_r, \sigma_r^2 \right),
\]

with

\[
\mu_r = \frac{2 \cdot \ln \left( 1 / \epsilon \right)}{s_l}, \quad \sigma_r = f_r \cdot \mu_r,
\]

where typically \( \epsilon = 0.1 \) and \( f_r = 0.4 \). For breaking the symmetry setting \( f_r > 0 \) is important. The detailed derivation of (17) will be presented in a separate paper.

Using the above method, we next initialize a network consisting of \( L = 170 \) layers with \( s_1 = 784 \) nodes in the input layer and \( s_l = 50 \) nodes in each consecutive layer. The input signal is uniformly distributed between 0 and 1.

The histograms of the first node in layer \( l = 50, l = 100 \) and \( l = 150 \) is depicted in Fig. 9.

![Fig. 9. Histograms of the first node in layer l = 50, l = 100 and l = 150.](image)

Although the variance of the activations is slightly decreasing with every layer, it is not vanishing until very late layers [5]. Furthermore no dying or saturated neurons are observed as is the case of ReLUs [11]. Same behaviour is observed for the backpropagated gradients \( s_j^{(l)} \) in (10).

8 Alternating Optimization Method

We discovered a technique, which improves the convergence in training deep neural networks (\( L > 50 \)) drastically. The trick is to optimize the sets of weights \( r_j^{(l)} \) and \( c_j^{(l)} \) for all nodes and all layers in an alternating way. For a certain number of iterations \( i_c \) during an epoch only weights \( r_j^{(l)} \) are optimized, while \( c_j^{(l)} \) are treated as constants. Then for a certain number of iterations \( i_r \) the opposite is done. Subsequently, the first step is repeated again and so on. As a finalization step in late epochs optionally a combined optimization can be performed. A positive side effect of applying the alternating optimization method lies in the reduced computational load.

9 Regularization

To help prevent overfitting, we make use of L2 regularization (also called a weight decay term). Since two sets of parameters are optimized in neural networks based on distance measures the overall cost function is of the form:

\[
J \left( R, C \right) = \frac{1}{m} \sum_{i=1}^{m} J \left( R, C; x^{(i)}, y^{(i)} \right)
\]

\[
+ \frac{\lambda_c}{2} \sum_{i=1}^{L} \sum_{j=1}^{s_i} \sum_{l=1}^{s_i+1} \left[ c_j^{(l)} \right]_i^2 + \frac{\lambda_r}{2} \sum_{i=1}^{L} \sum_{j=1}^{s_i} \sum_{l=1}^{s_i+1} \left[ r_j^{(l)} \right]_i^2
\]

where \( m \) denotes the number of samples in the training set and \( \lambda_c \) and \( \lambda_r \) are the regularization strengths. In general \( \lambda_c \) and \( \lambda_r \) have to be selected independently for getting optimal results. The second and third term in (18) tend to decrease the magnitude of the weights, and thus helps prevent overfitting.

Another way of preventing overfitting when using neural networks based on distance measures is to apply the alternating optimization method introduced in the previous section. Optimizing only for the half of the coefficients at each moment reduces the actual number of degrees of freedom, though acting as a form of regularization.
EXPERIMENTS

10.1 MNIST

In this subsection we demonstrate that the classification performance of the presented neural networks based on distance measures and Gaussian activation functions is comparable to the classification performance of traditional neural networks. To this end we use the well-known MNIST benchmark of handwritten digit images. MNIST consists of two datasets of handwritten digits of size 28x28 pixels, one for training (60,000 images) and one for testing (10,000 images). The goal of the experiment is not primarily to achieve state-of-the-art results, which would require convolutional layers and novel elastic training image deformations.

The input signal consists of raw pixel intensities of the original gray scale images mapped to real values pixel intensity range from 0 (background) to 1 (max foreground intensity). The dimension of the input signal is 28x28 = 784. The network architecture is built up of 2 fully-connected hidden layers with 100 units in each layer. We use the cross-entropy cost function in (7) and apply regularization (18) only to the radii terms, i.e. \( \lambda_c = 0 \). We use a variable learning rate that shrinks by a multiplicative constant after each epoch.

The test set accuracy after 30 epochs is 98.2%, which is a comparable result to a traditional neural networks with approx. the same number of parameters [4]. The weights of the first layer are depicted in Fig. 10 and Fig. 11.

Since neural networks in general are capable of approximating only continuous functions, the approximated image exhibits a blurry appearance. With a slightly increased number of layers and hidden units the approximation can be made indistinguishable from the original.

10.3 Approximating a probability density function

In the last example, we approximate a simple probability density function (pdf) consisting of a bivariate Gaussian distribution with a covariance matrix not being the identity matrix, i.e. a rotated Gaussian function, see. Fig. 13:

\[
  p_X(x) = \frac{1}{2\pi \sqrt{\det(\Sigma)}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu)^T \right) 
\]

where

\[
  \mu = \begin{pmatrix} -0.5 \\ 0.5 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 0.30 & 0.36 \\ 0.36 & 1.20 \end{pmatrix}.
\]

Since each layer in neural networks based on distance measures and Gaussian activation functions consists only of Gaussian functions aligned with the main axes (5), we want to see how well a minimal network consisting of 1 fully-connected hidden layer with 2 units is able to approximate this function. The result is depicted on the right hand side of Fig. 13. The approximation in the the vicinity of the peak is excellent. In the surrounding area a slight distortion is visible. The overall RMS of the approximation is 0.006.
11 CONCLUSIONS AND FUTURE WORK

In this paper, we have revisited neural network structures based on distance measures and Gaussian activation functions. We showed that training of these type of neural network is only feasible when using the stochastic gradient descent in combination with RMSProp. We showed also that with a proper initialization of the networks the vanishing gradient problem is much less than in traditional neural networks.

In our future work we will examine neural network architectures which are built up of combinations of traditional layers and layers based on distance measures and Gaussian activation functions introduced in this paper. In particular the use of layers based on distance measures in the output layer is showing very promising results. Currently we are analyzing the performance of neural networks based on distance measures when used in deep recurrent networks.

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