Understanding Dropout: Training Multi-Layer Perceptrons with Auxiliary Independent Stochastic Neurons

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Abstract. In this paper, a simple, general method of adding auxiliary stochastic neurons to a multi-layer perceptron is proposed. It is shown that the proposed method is a generalization of recently successful methods of dropout [5], explicit noise injection [12,3] and semantic hashing [10]. Under the proposed framework, an extension of dropout which allows using separate dropping probabilities for different hidden neurons, or layers, is found to be available. The use of different dropping probabilities for hidden layers separately is empirically investigated.

Keywords: Multi-layer Perceptron, Stochastic Neuron, Dropout, Deep Learning

1 Introduction

In this paper, we describe a simple extension to a multi-layer perceptron (MLP) that unifies some of the recently proposed training tricks for training an MLP. For example, the proposed extension is a generalization of using dropout for training an MLP [5].

The proposed method extends a conventional, deterministic MLP by augmenting each hidden neuron with an auxiliary stochastic neuron of which activation needs to be sampled. The activation of the added stochastic neurons is independent of all other variables in the MLP, and the weight of the edge connecting from the auxiliary neuron to the existing hidden neuron is fixed and not learned. Consequently, learning the parameters of the extended MLP does not require any special learning algorithm but can use a standard backpropagation [9].

This paper starts by briefly describing the proposed method of adding auxiliary stochastic neurons to an MLP. Then, it is described how dropout [5] and explicit noise injection [12,3] as well as semantic hashing [10] are all special cases of the proposed framework. Understanding the method of dropout under the proposed framework reveals that it is possible to use separate dropping probabilities for hidden neurons in a single MLP, and empirical investigation is provided on using different dropping probabilities for separate hidden layers.

2 Perceptron with Auxiliary Stochastic Neuron

For each hidden neuron $h_j^{[l]}$ in the l-th hidden layer, we introduce an independent stochastic neuron $r_j^{[l]}$ connected to $h_j^{[l]}$ with the edge weight $u_j^{[l]}$. The edge weight $u_j^{[l]}$

is *not* learned but fixed to a certain constant either indefinitely or for each forward computation¹.

The auxiliary stochastic neuron $r_j^{[l]}$ follows a predefined probability distribution, and its value is sampled at each evaluation of $h_j^{[l]}$. Since there is no incoming edge to the auxiliary neuron, the neuron is independent of any other variable in the MLP. In this case, the activation of the j-th hidden neuron in the l-th layer is

$$h_j^{[l]} = \phi \left(\sum_i h_i^{[l-1]} w_{ij}^{[l-1]} + r_j^{[l]} u_j^{[l]} \right),$$

where ϕ is a nonlinear function. $h_i^{[l-1]}$ and $w_{ij}^{[l-1]}$ are the i-th hidden neuron in the (l-1)-th hidden layer and the edge weight between $h_i^{[l-1]}$ and $h_j^{[l]}$, respectively. A hyperbolic tangent function $\tanh(\alpha)$ or a rectified linear function $\max(0,\alpha)$ is a common choice. See Fig. 1 for the illustration.

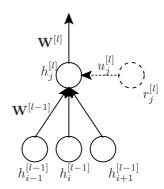


Fig. 1: Illustration of adding an auxiliary stochastic hidden neuron (marked by a dashed circle).

2.1 Learning and Prediction

It is straightforward to learn the parameters of this MLP. Since we do not attempt to learn $u_j^{[l]}$, a usual backpropagation [9] can be used. Only difference from the ordinary MLP which does not have auxiliary stochastic neurons is that the activations of the auxiliary neurons need to be sampled during the forward computation.

However, with a fixed set of parameters, either learned or predetermined by a user, it is not trivial to make a prediction given a new sample. Due to the stochastic activation of the auxiliary neurons, each forward computation of the output neurons will differ. A most obvious approach is to compute the output activation several times, and take the average or pick the most frequent one. This is however not preferred due to the increased computational cost as well as potentially high variance.

Another, more preferred way is to compute the expected activation of the output neurons over the distribution defined by the auxiliary stochastic neurons. This is often difficult as well due to the use of nonlinear activation functions. However, it is possible to linearize the computational path by approximating each nonlinear function linearly and push down the expectation operator to each auxiliary neuron. One can, then, compute and use the approximate expected activation of the output neurons as the final prediction.

¹ The author acknowledges that a similar method of a hidden neuron having an independent noise source, called a *semi-hard stochastic neuron*, has been recently proposed in [1] independently of this work.

3 Understanding Dropout with Auxiliary Stochastic Neurons

A dropout is a regularization technique which forces the activations of a randomly selected half of hidden neurons in each layer to zero when training an MLP. Just like the proposed method of adding auxiliary stochastic neurons training an MLP with dropout changes the forward computation only and leaves the error backpropagation as it is.

3.1 Training

Let us consider an MLP using rectified linear hidden neurons. Then, learning with dropout is equivalent to training an MLP with auxiliary stochastic neurons of which each follows Bernoulli distribution with mean p=0.5. We fix the weight $u_j^{[l]}$ of the edge connecting from the auxiliary stochastic neuron to a hidden neuron to negative infinity. Then, the activation of $h_j^{[l]}$ is

$$h_j^{[l]} = \begin{cases} \max(0, \alpha_j^{[l]}), & \text{if } r_j^{[l]} = 0\\ 0, & \text{if } r_j^{[l]} = 1 \end{cases}$$
 (1)

This is equivalent to using dropout in training an MLP.

This exact procedure applies to any hidden neuron which has an activation function that converges to zero in the limit of negative infinity. A logistic sigmoid activation function is one such example. In cases of other types of activation functions, other ways of fixing the connection strengths between a hidden neuron and its corresponding auxiliary neuron are needed.

3.2 Testing

When an MLP was trained using a procedure of dropout, it was proposed in [5] that outgoing weights be halved to compensate for the loss of approximately half of hidden neurons during training phase. With a mild approximation, here we show that this procedure of halving the outgoing weights corresponds to computing the expected activation of output neurons over the auxiliary stochastic neurons.

If we linearly approximate the expectation of the output neurons, we may push the expectation operator all the way down to the evaluation of the activation of each hidden neuron $h_j^{[l]}$. Because the activation is dropped to zero with probability 0.5, the expected activation of $h_j^{[l]}$ becomes, for instance in the case of a rectified linear hidden neuron in Eq. (1),

$$\mathbb{E}\left[h_j^{[l]}\right] = \frac{1}{2} \max\left(0, \sum_i h_i^{[l-1]} w_{ij}^{[l-1]}\right).$$

It is clear to see that this is effectively equivalent to halving the outgoing weights.

Linear approximation is unnecessary, and computing the expectation becomes exact, if the output neurons are linear and there is only a single layer of hidden neurons. This agrees well with the original formulation of dropout in [5] which formulated the

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procedure of halving the outgoing weights as taking a geometric average of exponentially many neural networks that share parameters. However, this procedure, in both perspectives, becomes approximate as the number of nonlinear hidden layers increases.

From the proposed framework, we can see that, albeit informally, this procedure of halving the outgoing weights is well approximated if the activation function of each hidden neuron can be approximated well linearly. There are two potential consequences from this. Applying dropout to hidden neurons below an activation function which may not be well approximated linearly, such as max-pooling, will not work well, which has been noticed already by previous work (see, e.g., [14,6]). Secondly, a piece-wise linear activation function such as the rectified linear function is well-suited for using dropout. This agree well with recent finding that another piece-wise linear activation function called maxout works well with dropout [4].

By this formulation, we can extend the original dropout by dropping each hidden neuron with probability p instead of 0.5. In that case, in testing time, the outgoing weight will be multiplied by 1-p. Furthermore, this allows us to use different dropping probabilities for hidden neurons. If we denote the dropping probability of each hidden neuron by $p_j^{[l]}$, this will correspond to multiplying all outgoing weights $w_{jk}^{[l]}$ of the j-th hidden neuron in the l-th hidden layer with $1-p_j^{[l]}$.

4 Other Special Cases

In this section, we describe two other popular training schemes and how they are realized as special cases of the proposed procedure of adding auxiliary stochastic neurons. The two training schemes we discuss here are denoising [12,3] and semantic hashing [10].

4.1 Explicit Noise Injection: Denoising Autoencoder

A denoising autoencoder (DAE) [12] is an MLP that aims to reconstruct a clean sample given an explicitly corrupted input. The DAE is an obvious special case of the proposed general framework. In this section, we consider adding additive white Gaussian noise to each input component.

A DAE can be constructed from an ordinary autoencoder by adding an additional hidden layer between the input and the first hidden layer. The additional layer has as many hidden neurons as the number of input variables. Each hidden neuron ν_i is connected to the i-th input component x_i only with weight 1 and has an auxiliary stochastic neuron r_i which follows a standard Normal distribution.

The activation of ν_i is linear and defined to be

$$\nu_i = x_i + r_i u_i,$$

where u_i is the connection strength between ν_i and r_i . Each time ν_i is computed, the activation of r_i is sampled from a standard Normal distribution. This is equivalent to explicitly adding additive white Gaussian noise with variance r_i^2 .

Once training is over, we can compute the hidden activation of the original DAE by first computing the expected activation of ν_i . Since $\mathbb{E}\left[r_i\right]=0$, the activation of ν_i is simply a copy of the input x_i . In other words, we can use the learned parameters as if they were the parameters of an ordinary autoencoder trained without explicitly adding noise.

By further adding more intermediate hidden layers with auxiliary stochastic neurons, we can emulate adding multiple types of noise sequentially to input. For instance, a common practice of adding white Gaussian noise and dropping a small portion of input components can be achieved by adding another intermediate hidden layer that drops some components randomly, just like dropout described in Section 3.

This method of explicitly injecting noise to input is obviously applicable to a standard MLP that performs classification [3,8]. Furthermore, under the proposed framework this method naturally allows us to add noise even to hidden neurons, which may work as a regularization similarly to using dropout. This idea of adding noise to hidden neurons as well as input variables has recently been applied to a deep generative stochastic network in [2].

4.2 Semantic Hashing

Semantic hashing was proposed in [10] to extract a binary code of a document using a deep autoencoder with a small sigmoid bottleneck layer. One of the important details of the training procedure in [10] was to add white Gaussian noise to the input signal to the bottleneck layer to encourage the activations of the hidden neurons in the bottleneck layer to be as close to 0 or 1 as possible.

This procedure is exactly equivalent to adding an auxiliary stochastic neuron to each bottleneck hidden neuron. The activation of each auxiliary stochastic neuron is sampled from a standard Normal distribution and is multiplied with the connection strength which corresponds to the variance of the added noise. Since the connection strength is fixed and the auxiliary stochastic neuron is independent from the input or any other neuron, an ordinary backpropagation can be used without any complication resulting from the stochastic auxiliary neurons.

Again, once the parameters were learned, one may safely ignore the added auxiliary stochastic neurons as their means are zero.

5 Experiments

Although this paper focuses on interpreting various recently proposed training schemes under the proposed framework of adding auxiliary stochastic neurons. We were able to find some potentially useful extensions of those existing schemes by understanding them from this new perspective. One of them is to extend the usage of dropout by using different dropping probabilities for hidden neurons, and another is to inject white Gaussian noise to hidden neurons.

In this section, we present preliminary experiment result showing the effect of (1) using a separate dropping probability for each hidden layer and (2) injecting white Gaussian noise to the *input* of each hidden neuron.

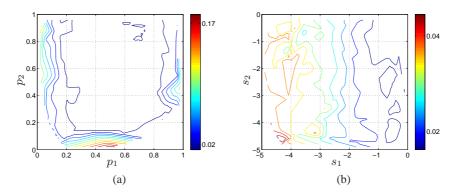


Fig. 2: Contour plots of interpolated classification errors. (a) Figure obtained by the MLPs trained using separate dropping probabilities p_1 and p_2 for two hidden layers. (b) Figure obtained by the MLPs trained by injecting white Gaussian noise to the inputs to hidden neurons using separate standard deviations s_1 and s_2 for two hidden layers. These figures are best viewed in color.

5.1 Settings

We trained MLPs with two hidden layers having 2000 rectified linear neurons each on handwritten digit dataset (MNIST, [7]) using either dropout with separate dropping probabilities for the two hidden layers or injecting white Gaussian noise.

To see the effect of choosing separate dropping probabilities for hidden layers, we trained 100 MLPs with a dropping probability p_l with the l-th hidden layer randomly selected from the interval [0,1]. Similarly, 100 MLPs were trained with separate noise variances for hidden layers, where the exponent s_l of a noise variance for the l-th hidden layer was randomly chosen from [-5,0].

Before training each MLP, 60,000 training samples were randomly split into training and validation sets with ratio 3:1. Learning was early stopped by checking the prediction error on the validation set, while the maximum number of epochs was limited to 100^2 . We used a recently proposed method, called ADADELTA [13], to adapt learning rates automatically. Since we fixed the size of an MLP, this effectively means that there were no other hyperparameters to tune.

5.2 Result and Analysis

The result for the first experiment tested using separate dropping probabilities for hidden layers is shown in Fig. 2 (a). Interestingly, it can be observed that any dropping probability near 0.5 resulted in relative good accuracy. However, when any extreme dropping probability close to either 0 or 1 was used for the first hidden layer (p_1) , the performance dropped significantly regardless of the dropping probability of the second hidden layer (p_2) . Using too small dropping probability in the second hidden layer also turned out to hurt the generalization performance significantly. This suggests that

² Almost all runs were early-stopped before 100 epochs.

the original proposal of simply dropping approximately half of hidden neurons in each hidden layer from [5] is already a good choice.

In Fig. 2 (b), the result of the second experiment is shown. In general, it shows that the generalization performance of an MLP is highly affected by the level of noise injected at the first hidden layer, which is in accordance with the previous research showing that adding noise to the input improves the classification accuracy on test samples [8]. However, a closer look at the figure shows that adding noise to the upper hidden layer helps achieving better generalization performance (see the upper right corner of the figure).

One important lesson from these preliminary experiments is that it is possible to achieve better generalization performance by carefully tuning auxiliary stochastic neurons. This amounts to, for instance, choosing different dropping probabilities in the case of dropout and injecting different levels of Gaussian noise. Further and deeper investigation using various architectures and datasets is, however, required.

6 Discussion

In this paper, we have described a general method of adding auxiliary stochastic neurons in a multi-layer perceptron (MLP). This procedure effectively makes hidden neurons in an MLP stochastic, but does not require any change to the standard backpropagation algorithm which is commonly used to train an MLP.

This proposed method turned out to be a generalization of a few recently introduced training schemes. For instance, dropout [5] was found to be a special case having binary auxiliary neurons with connection strengths dependent on the input signal. A method of explicitly injecting noise to input neurons [3,8] used by, for instance, a denoising autoencoder [12] was found to be an obvious application of the proposed use of auxiliary stochastic neurons following standard Normal distribution. Furthermore, we found that a trick of making the activations of hidden neurons in the bottleneck layer of an autoencoder used for semantic hashing [10] is equivalent to simply adding a white Gaussian auxiliary stochastic neuron to each hidden neuron in a bottleneck layer.

This paper, however, did not attempt to explain why, for instance, dropout helps achieving better generalization performance. Training an MLP with dropout under the proposed framework does not differ greatly from the ordinary way of training. The only difference is that some randomness is explicitly defined and injected via auxiliary stochastic neurons. It is left for future to investigate whether this simple injection of randomness causes a favorable performance of an MLP trained with dropout, or there exist more behind-the-scene explanations. The same argument applies to denoising autoencoders and semantic hashing as well.

One important thing to note is that the proposed method is *not* equivalent to building an MLP with stochastic activation functions. It may be possible to find an equivalent model with auxiliary stochastic neurons, but it is not guaranteed nor expected that every stochastic MLP can be emulated by an ordinary MLP augmented with auxiliary stochastic neurons. However, one advantage of using the proposed method of adding auxiliary neurons compared to a true stochastic MLP is that there is no need for mod-

ifying the standard backpropagation or designing a new learning algorithm (see, e.g., [1,11]).

By understanding the method of dropout under the proposed framework, another extension was found, which allows using a separate dropping probability for each hidden layer. Similarly, we observed that it is also possible, under the proposed framework, to inject white Gaussian noise at each hidden layer instead of injecting only at the input. In the experiments, we provided empirical evidence showing that better generalization performance may be achieved by using separate dropping probabilities for different hidden layers in the case of dropout as well as injecting white Gaussian noise to hidden layers. As the experiments were quite limited, however, further extensive evaluation is required in future.

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