ProbAct: A Probabilistic Activation Function for Deep Neural Networks

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Abstract

Activation functions play an important role in the performance and generalization of a deep neural network. Though majority of the activation functions are deterministic, we propose a novel probabilistic activation function, called ProbAct. ProbAct is decomposed into a mean and variance and the output value is sampled from the formed distribution, making ProbAct a stochastic activation function. The values of mean and variances can be fixed using known functions or trained for each element. In the trainable ProbAct, the mean and the variance of the activation distribution is trained within the back-propagation framework alongside other parameters. We show that the stochastic perturbation induced through ProbAct acts as a viable generalization technique for feature augmentation. In our experiments, we compare ProbAct with well-known activation functions on classification tasks on different modalities: Images (CIFAR-10, CIFAR-100 and STL-10) and Text (Large Movie Review). We show that ProbAct increases the classification accuracy by +2-3% compared to ReLU or other conventional activation functions on both original datasets and when datasets are reduced to 50% and 25% of the original size.

1. Background

Activation functions add non-linearity to neural networks which helps them learn complex functional mappings from data [24]. Research on activation functions can be broadly separated into two approaches: fixed activation functions, and adaptive activation functions. Fixed activation functions are constant pre-determined functions such as Sigmoid [7], hyperbolic tangent (Tanh), the Rectified Linear Unit (ReLU) [19] and its variants e.g., Leaky ReLU [27], Parametric ReLU (PReLU) [11], and Exponential Linear Unit (ELU) [4] among several others. Adaptive activation functions use trainable parameters in order to optimize the activation function like Parametric ReLUs (PReLU) [11] with a trainable parameter instead of a fixed value. However, all of these are deterministic activation
functions with fixed input-output relationships. In this work, we propose a new activation function, called \textit{ProbAct}, which is not only trainable but also stochastic in nature. For the same input value \( x \), the output value from \textit{ProbAct} varies stochastically — a capability conventional activation functions do not offer.

There has been a lot of work on adding noise to the activation function, mainly to prevent network overfitting. Noisy activation functions \cite{10} add noise in proportion to the magnitude of saturation of the non-linearity. However, for \cite{10}, the \( \sigma \) is dependant on the difference between the activation function and its linearization. The exact relationship between them was achieved through intensive experimentation. Our method requires no such computation as the mean and variance are learned as the part of network parameters. \cite{20} shows that training with regularization by noise is equivalent to optimizing the lower bound of the marginal likelihood. For training, a set of noise samples is drawn and forward and backward propagation for each noise sample is performed to estimate the likelihoods and the corresponding gradients. This requires setting up the mean and variance for each run, whereas our method learns the mean and variance during training. To demonstrate that \textit{ProbAct} is not equivalent to just adding noise to the activations, we compared \textit{ProbAct} with \textit{ReLU activation} with Gaussian noise and with \textit{noisy inputs}.

Furthermore, the effect of adding noise to weights, by considering weights as a distribution \cite{1, 3, 8, 9, 12, 18, 22, 26} have been studied. All these methods learn distribution over weights either by approximating the true posterior or considering the last layers as distributions. Our case differs from these works by learning distributions over the activation function. Our variance is input-independent while \cite{8, 12, 26} produce input-dependent variance, making \textit{ProbAct} faster and less computationally expensive.

2. \textbf{ProbAct: A Stochastic Activation Function}

Every layer of a neural network computes its output \( y \) for the given input \( x \):

\[
y = f(w^T x),
\]

where \( w \) is the weight vector of the layer and \( f(\cdot) \) is an activation function, such as \textit{ProbAct}. \textit{ProbAct} is defined as:

\[
f(a) = \mu(a) + \sigma \epsilon,
\]
where, \( a \) is the input to the activation function, \( \mu(a) \) is a static or learnable mean (for example, \( \mu(a) = \max(0, a) \) if it is static ReLU) and the perturbation parameter \( \sigma \) is a fixed or trainable value which specifies the range of stochastic perturbation and \( \epsilon \) is a random value sampled from a normal distribution \( \mathcal{N}(0, 1) \). The value of \( \sigma \) is either determined manually or trained along with other network parameters (i.e., weights) with simple implementation. With decreasing \( \sigma \), ProbAct converges to its mean function \( \mu(a) \). If \( \sigma \rightarrow 0 \), ProbAct behaves the same as its mean function. Example: if the mean is a fixed ReLU function, then ProbAct acts a generalization of ReLU in that case.

2.1. Setting the Parameter for Mean

The mean function \( \mu(a) \) is trained for every input \( a \), i.e. element-wise. However, learning the mean value with zero or random initialization takes unnecessarily long to converge. So, we propose initialization of \( \mu(a) \) with known functions such as ReLU with \( \mu(a) = \max(0, a) \). Besides ReLU, any known functions can be used as an initializer. We use ReLU for its simplicity and good convergence behavior.

2.2. Setting the Parameter for Stochastic Perturbation

The parameter \( \sigma \) specifies the range of stochastic perturbation. In the following, we will consider two cases of setting \( \sigma \), fixed and trainable.

**Fixed Case** There are several ways to choose the desired \( \sigma \). The simplest is setting \( \sigma \) to be a constant hyper-parameter. Choosing one constant \( \sigma \) for all elements is theoretically justified as \( \epsilon \) is randomly sampled from a normal distribution \( \mathcal{N}(0, 1) \), and \( \sigma \) acts as a scaling factor to the sampled value \( \epsilon \). This can be interpreted as repeated addition of the scaled Gaussian noise to the activation maps, which helps in better convergence of the network parameters [2]. The network is optimized using gradient-based learning. The proposed method does not significantly affect the number of parameters in the architecture, hence comes at no additional computational cost.

**Trainable Case** Using a trainable \( \sigma \) reduces the requirement to determine \( \sigma \) as a hyper-parameter and allows the network to learn the appropriate range of sampling. There are two ways of introducing a trainable \( \sigma \):

- **Single Trainable \( \sigma \)**: A shared trainable \( \sigma \) across the network. This introduces a single extra parameter used for all ProbAct layers. This is similar to the fixed \( \sigma \) but the value is trained.

- **Element-wise Trainable \( \sigma \)**: This method uses a trainable parameter for each input element. This adds the flexibility to learn a different distribution for every input-output mapping.

3. Experiments

In the experiments, we empirically evaluate ProbAct on image classification and sentiment analysis tasks to show the effectiveness of the proposed method. We use three image classification datasets, CIFAR-10 [15], CIFAR-100 [15], and STL-10 [6] and one text dataset: Large Movie Review [17]. More information on the dataset distribution is mentioned in the Appendix.

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1. Results taken from this implementation:
   https://github.com/kumar-shridhar/PyTorch-BayesianCNN
Figure 2: (a) and (b) shows the test accuracy comparison between ReLU and ProbAct layer with/without dropout layers on CIFAR-10 and CIFAR-100 datasets respectively. (c) shows the test accuracy comparison between ReLU with noisy input and ProbAct, and (d) shows the test accuracy comparison of ReLU, ReLU with noisy activation and ProbAct on CIFAR-10 dataset.

Table 1: Performance comparison of various activation functions and a Variation Inference Neural Network with ProbAct. The test accuracy(%) indicates the average of testing over three runs. The train and test time is reported with respect to ReLU activation function and is measured in seconds and milliseconds respectively.

| Activation function  | CIFAR-10 | CIFAR-100 | STL-10 | IMDB | Train time (sec) | Test time (milli-sec) |
|----------------------|----------|-----------|--------|------|------------------|---------------------|
| Sigmoid              | 10.00    | 1.00      | 10.00  | 85.92| 1.07             | 1.03                |
| Tanh                 | 10.00    | 1.00      | 10.00  | 85.88| 1.08             | 1.03                |
| ReLU                 | 87.27    | 52.94     | 60.80  | 85.85| 1.00             | 1.00                |
| Leaky ReLU           | 86.49    | 49.44     | 59.16  | 85.47| 1.04             | 1.08                |
| PReLU                | 86.35    | 46.30     | 60.01  | 85.95| 1.16             | 1.00                |
| ELU                  | 87.65    | 56.60     | 64.21  | 86.51| 1.16             | 1.04                |
| SELU                 | 86.65    | 51.52     | 60.71  | 85.71| 1.19             | 1.05                |
| Swish                | 86.55    | 54.01     | 63.50  | 86.14| 1.20             | 1.13                |
| Bayesian VGG VI      | 86.22    | 48.27     | 57.22  | -    | -                | -                   |
| ProbAct Mean         | 85.80    | 48.50     | 54.17  | 83.86| 1.29             | 1.35                |
| Element-wise $\mu$  | 88.87    | 58.45     | 62.50  | 87.31| 1.10             | 1.27                |
| Fixed ($\sigma = 0.5$) | 88.40    | 53.87     | 63.07  | 86.35| 1.23             | 1.30                |
| One Trainable $\sigma$ | 86.40    | 54.10     | 61.70  | 86.64| 1.25             | 1.31                |
| EW Trainable $\sigma$ | 88.92    | 55.83     | 64.17  | 85.86| 1.26             | 1.33                |

3.1. Experimental Setup

To evaluate the performance of the proposed method on classification tasks, we compare ProbAct to the following activation functions: ReLU, Sigmoid, Hyperbolic Tangent (TanH), Leaky ReLU [27], PReLU [11], ELU [5], SELU [14], Swish [21] and to a Bayesian VGG network using variational inference [16]. We utilize a 16-layer VGG neural network [23] architecture for the image classification task and a two-layer CNN network for sentiment analysis task. The architecture, specific hyper-parameters, and training settings are provided in the Appendix section.

For a fair and consistent evaluation environment, we did not use regularization tricks, pre-training, and data augmentation to show the true comparison of the activations. The inputs are normalized to $[0, 1]$. The STL-10 images are resized to 32 by 32 to match the CIFAR datasets to keep a fixed input shape to the network.

When using Element-wise Trainable $\sigma$ (bound) ProbAct, we achieved performance improvements of 2.25% on CIFAR-10, 2.89% on CIFAR-100, 3.37% on STL-10, and 1.5% on IMDB datasets.
Table 2: Test Accuracy (%) comparison between ReLU and ProbAct on reduced subsets of CIFAR-10 and CIFAR-100 (50% and 25% of original dataset). The test accuracy(%) indicates the average of three sets of testing.

| Activation function | CIFAR-10 (50%) | CIFAR-100 (50%) | CIFAR-10 (25%) | CIFAR-100 (25%) |
|---------------------|----------------|-----------------|----------------|-----------------|
| ReLU                | 82.74          | 42.36           | 75.62          | 30.42           |
| ProbAct             | **84.73**      | **46.11**       | **79.02**      | **31.67**       |

compared to the standard ReLU. In addition, the proposed method performed better than any of the evaluated activation functions. We did not see any improvements while training both \( \mu \) and \( \sigma \) together as their individual accuracy is similar and merging the two modalities did not help. However, training them individually have their own advantages as mentioned in the next section.

In order to demonstrate the applicability of our proposed method, the training and testing times relative to the standard ReLU are also shown in Table 1. The time comparison shows that we can achieve higher performance with only a relatively small time difference. This is mainly because the learnable \( \sigma \) values are few compared to the learnable weight values in a network. Hence, our approach comes at nearly no additional time cost. This shows ProbAct as a strong replacement over popular activation functions.

3.2. Augmentation by Activation

We add ProbAct to the first layer of the VGG network keeping ReLU as the activation function for all the other layers. We show that perturbation induced by ProbAct in the first layer behaves as augmentation added in the activation function; improving the overall network generalization ability. ProbAct can be thought of as a way to add an adaptable and trainable perturbation enhancing the generalization capability of the network. These added perturbations are different than just adding noise to either the activation or to the inputs. Figure 2 (c) draws a comparison between ProbAct in the first layer with noisy input (in our experiments, Gaussian noise was added to the inputs sampled from a distribution \( \mathcal{N}(0, 1) \)), while in Figure 2 (d), Gaussian noise is added to the first activation layer. ProbAct with learnable variance outperforms both the standard ReLU with noisy inputs and standard ReLU with noisy activations. Our proposed method adopts stochastic noise into the activation function in a controlled manner.

3.3. Reduced Data

The training sample size was reduced to 50% and 25% of the original data size for CIFAR-10 and CIFAR-100 dataset. We maintained the class distribution by randomly choosing 25% and 50% images for each class. The process was repeated three times to create three randomly chosen datasets. We run our experiments on all three datasets and average the results.

Table 2 shows the test accuracy for ReLU and ProbAct with Element-wise Trainable \( \sigma \) (bound) on 25% and 50% data size. We achieve 3% average increase in test accuracy when the data size was halved and 2.5% increase when it was further halved. The higher test accuracy of ProbAct shows the applications of ProbAct in real-life use cases when the training data size is small.
4. Conclusion

In this paper, we introduce a novel probabilistic activation function, ProbAct, which adds perturbation in every activation map, allowing better network generalization capabilities. We verified empirically that the stochastic perturbation prevents the network from memorizing the training samples, resulting in evenly optimized network weights and a more robust network with a lower generalization error. Furthermore, we confirmed that the augmentation-like operation in ProbAct is effective for classification tasks even when the number of data points is very low.

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5. Appendix

The VGG-16 architecture used in the experiments is defined as follows:

\[
\text{VGG16 : [64, 64, M, 128, 128, M, 256, 256, 256, M, 512, 512, 512, M, 512, 512, 512, M, C]}
\]

where, numbers 64, 128 and 256 represents the filters of Convolution layer which is followed by a Batch Normalization layer, followed by an activation function. \( M \) represents the Max Pooling layer and \( C \) represents the Linear classification layer of dimension (512, number of classes).

Other hyper-parameters settings include:

| Hyper-parameter                        | Value                        |
|----------------------------------------|------------------------------|
| Convolution Kernel Size                | 3                            |
| Convolution layer Padding              | 1                            |
| Max-Pooling Kernel Size                | 2                            |
| Max-Pooling Stride                     | 2                            |
| Optimizer                              | Adam                         |
| Batch Size                             | 256                          |
| Fixed \( \sigma \) values              | [0.05, 0.1, 0.25, 0.5, 1, 2] |
| Learning Rate                          | 0.01 (Dropped 1/10 after every 100 epochs) |
| Number of Epochs                       | 400                          |
| Image Resolution                       | \(32 \times 32\)            |
| Single trainable \( \sigma \) Initializer | Zero                       |
| Element-wise trainable \( \sigma \) Initializer | Xavier initialization |

5.1. Datasets

5.1.1. IMAGE DATASETS

**CIFAR-10 Dataset**  The CIFAR-10 dataset consists of 60,000 images with 10 classes, with 6,000 images per class, each image 32 by 32 pixels. The dataset is split into 50,000 training images and 10,000 test images.

**CIFAR-100 Dataset**  CIFAR-100 dataset has 100 classes containing 600 images per class. There are 500 training images and 100 test images per class. The resolution of the images is also 32 by 32 pixels.

**STL-10 Dataset**  STL-10 dataset has 500 images per class with 10 classes and 100 test images per class. The images are 96 by 96 pixels per image.

5.1.2. TEXT DATASET

**Large Movie Review Dataset**  Large Movie Review [17] is a binary dataset for sentiment classification (positive or negative) consisting of 25,000 highly polar movie reviews for training, and 25,000 reviews for testing.
5.2. Proofs

Theorem 1 The gradient propagation of a stochastic unit $h$ based on a deterministic function $g$ with inputs $x$ (a vector containing outputs from other neurons), internal parameters $\phi$ (weights and bias) and noise $z$ is possible, if $g(x, \phi, z)$ has non-zero gradients with respect to $x$ and $\phi$. [2]

$$h = g(x, \phi, z) \quad (3)$$

Assume a network has two layers with a unit for each layer, the distribution of the second layer’s output $y_2$ differs depending on the first and second layer’s weights ($w_1$ and $w_2$) and sigmas ($\sigma_1$ and $\sigma_2$) as:

$$y_2 = \mu [w_2 \mu(w_1 x) + w_2 \sigma_1 \epsilon] + \sigma_2 \epsilon$$

$$= \begin{cases} 
\mu [w_2 \mu(w_1 x)] + w_2 \sigma_1 \epsilon + \sigma_2 \epsilon & \text{if } w_2 \mu(w_1 x) + w_2 \sigma_1 \epsilon > 0, \\
\sigma_2 \epsilon & \text{otherwise},
\end{cases}$$

$$\sim \begin{cases} 
N(\mu [w_2 \mu(w_1 x)], (w_2 \sigma_1)^2 + \sigma_2^2) & \\
N(0, \sigma_2^2).
\end{cases} \quad (4)$$

Incidentally, as shown in Figure 1 (c) in the main paper, a small noise variance tends to be learned in the final layer to make the network output stable (see Section 4.3 in the paper for a quantitative evaluation).

Using Eq. (3) from Theorem 1, assume $g$ is noise injection function that depends on noise $z$, and some differentiable transformations $d$ over inputs $x$ and model internal parameters $\phi$. We can derive the output, $h$ as:

$$h = g(d, z) \quad (5)$$

If we use Eq. (5) for another noise addition methods like dropout [13] or masking the noise in denoising auto-encoders [25], we can infer $z$ as noise multiplied just after a non-linearity is induced in a neuron. In the case of ProbAct, we sample from Gaussian noise and add it while computing $h$. Or we can say, we add a noise to the pre-activation, which is used as an input to the next layer. In doing so, self regularization behaviour is induced in the network.
Figure 3: Comparison of predictive test accuracy and confidence score between ReLU (above) and ProbAct (below) on a VGG-16 architecture on CIFAR-10 dataset with 0.05 Gaussian noise added to test samples.

Figure 4: (a) Comparison of different mean settings with fixed $\sigma = 1$ for CIFAR-10 datasets. Channel-Wise mean denotes a constant learnable mean within the channels, element-wise mean denotes learnable mean for each parameter, while one mean denotes a single learnable mean for entire dataset. It is worth noting that element-wise mean takes a lot more time to converge compared to one mean or channel-wise mean. This shows that using single learnable mean uses fewer parameters and converges faster.(b) denotes the different variance settings for CIFAR-10 dataset. On contrary to mean settings, there is no clear convergence time difference between single variance and channel-wise variance. Single variance is preferred due to the usage of fewer parameters.Training element-wise mean and element-wise variance (denoted as EW) leads to too many learnable parameters and takes a long time to converge. Training time is high for such a solution and is only preferred when overfitting is an issue.
Figure 5: Different mean and variance setting of ProbAct for CIFAR-100 dataset. It is worth noting that single learnable mean is equally effective compared to channel-wise learnable mean but with fewer parameters. Element-wise mean accuracy is lesser than the others but it is more susceptible to overfitting as stated in the paper.

Figure 6: (a) and (b) shows the train and test accuracy comparison between ReLU and ProbAct layer with/without dropout layers on CIFAR-100 dataset. With $\sigma = 2$, ProbAct achieves similar test performance to ReLU activation layer with dropout with less overfitting as shown from the training curve. Adding a dropout layer further improves the generalization capabilities, showing the built-in regularization nature of ProbAct.