Evolving Neural Selection with Adaptive Regularization

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ABSTRACT

Over-parameterization is one of the inherent characteristics of modern deep neural networks, which can often be overcome by leveraging regularization methods, such as Dropout [31]. Usually, these methods are applied globally and all the input cases are treated equally. However, given the natural variation of the input space for real-world tasks such as image recognition and natural language understanding, it is unlikely that a fixed regularization pattern will have the same effectiveness for all the input cases. In this work, we demonstrate a method in which the selection of neurons in deep neural networks evolves, adapting to the difficulty of prediction. We propose the Adaptive Neural Selection (ANS) framework, which evolves to weigh neurons in a layer to form network variants that are suitable to handle different input cases. Experimental results show that the proposed method can significantly improve the performance of commonly-used neural network architectures on standard image recognition benchmarks. Ablation studies also validate the effectiveness and contribution of each component in the proposed framework.

CCS CONCEPTS

• Computing methodologies → Neural networks;

KEYWORDS

Neural Networks, Selection Methods, Neural Evolution

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1 INTRODUCTION

Modern neural networks usually adopt deep architectures with millions of parameters and connections. One common issue with such designs is over-parameterization [24], in which case the number of parameters is too large for the task. This situation often results in overfitting, which hurts the generalization capability of the model at test time, as the deep network tends to learn specific representations and memorize all the training samples. A general strategy to resolve this problem is to use regularization methods that penalize the model using too many parameters. For neural networks specifically, Dropout [31] has been a common method which randomly selects a certain ratio of neurons from a layer of the network and temporarily removes them along with all their incoming and outgoing connections. For every training iteration the network will use fewer parameters in a probabilistic fashion, and thus can be prevented from learning specific representations for each training sample.

There are a number of studies proposing variants of Dropout that impose certain structures to specific models or tasks. However, most of them are highly specialized and can not be easily adapted to different network architectures or training protocols. In the image recognition domain, the most common way of using Dropout is to apply it to the fully-connected layers or simply the last fully-connected layer before the classification layer. Some recent studies also propose variants that perform Dropout on convolutional layers by dropping neurons in particular structures. For example, DropPath [39] forms multi-branched convolutional cells and drops one random branch each time. DropBlock [8] selects contiguous squares of neurons in the convolutional layers and drops them. However, these methods usually require specific tuning of the architecture and parameters based on the model and dataset. In other words, the same dropout pattern does not work as well on a different model or dataset. More recently, AutoDropout [27] proposes to automate the process of designing dropout patterns in a reinforcement learning setting. While it shows promising improvement over numerous benchmarks, the cost of searching dropout patterns can be over a magnitude higher than the training job itself, making the method less practical in real-world tasks.

In general, the main idea of these previous works is, while neural networks usually show better performance when going deeper and having more parameters (assuming that there exists a sufficiently large amount of data), they are not necessarily required to use all the neurons to make good predictions, i.e., the activation units in a layer can be sparse. Such sparsity in practice has a regularization effect on over-parameterization. However, most previous works tend to explore specific ways to apply regularization, and use the same regularization pattern over all the input training samples, which may not be optimal because the complexity and variation of input samples are essentially different. For example, distinguishing images of coarse categories, such as dogs vs. cats, is much easier than distinguishing more fine-grained categories, such as two certain species of dogs, because the latter requires learning a more complex combination of visual representations. Thus, another potential way to improve regularization in deep neural networks is to properly allocate the right number of neurons based on each input
case, and such a number is just enough for the model to make a correct prediction.

In this work, we aim to explore this regime of keeping essential neurons and dropping out unnecessary ones based on the input data, in order to form simple and powerful representations that generalize well to unseen test cases. An alternative way to view this goal is to generate different network variants that are selected to handle each input sample accordingly, because the samples are likely to require different numbers of neurons to form reasonable representations. Inadequate resources may cause undermined model performance, and on the other hand, overwhelming resources are likely to make the model overfit. As similar problems are well studied in the literature of evolutionary computing [6], we consider a novel strategy that evolves selections of neurons to form neural network variants in parallel with the training process of the neural network. The fitness of each network variant is measured by the model performance and the number of neurons used for the prediction. We term this framework Adaptive Neural Selection (ANS), which consists of two parts: a self-attention module and an adaptive regularization mechanism.

The self-attention module is intended to perform selection of neurons by learning a variable weight to be imposed on each neuron. The attention mechanism has been shown in several previous studies [4, 12, 34] to help deep networks focus on essential features and neurons. While the self-attention module can be trained end-to-end in parallel with the neural network through gradient descent, it does not have an objective to adapt neural selection based on the difficulty of predicting each input sample. Thus, we further introduce an adaptive regularization method. This regularization works as a selection pressure that penalizes the self-attention module if it is selecting more neurons than required. The penalization is adaptive to different training samples in regard to the difficulty of performing the task. For example, given a batch of images, if the classification accuracy is low, that means the model has not fully learned good representations of these cases, and thus it is allowed to use more neurons to explore a more complex feature space. The two mechanisms work together to form the Adaptive Neural Selection (ANS) framework, which evolves different sub-network variants by learning the adaptive selection of neurons. ANS can be used on any neural network architecture to adapt its complexity and structure to handle the variety of input cases.
We implement the proposed ANS framework and test it for the image classification task, which is one of the most common tasks for modern deep neural networks. The experiments show that ANS significantly improves commonly-used deep ConvNet architectures on standard benchmarks. On CIFAR-100, ANS improves the test accuracy of ResNet-50 from 76.65% to 78.08%, and VGG-16 from 62.30% to 65.21%, outperforming Dropout [31] by a significant margin. Ablation studies also validate that the two components both make a good contribution to the improvement.

In the following sections, we first summarize the related work in the area of machine learning and evolutionary computing. Then we describe the ANS framework and its components. This is followed by experimental results showing the performance of our method. Finally, we conclude by summarizing the results and listing directions for future work.

2 RELATED WORK

Within the broader context of machine learning research, this paper is in line with existing works on regularization methods for neural networks [5, 7, 8, 13, 24, 27, 31, 36, 39]. Most of the recent methods such as Dropout [31] and its variants require either specific and careful tuning of the structure based on the datasets or tasks [8, 39], or expensive computation cost for searching good patterns of regularization [27]. Instead of expanding on the current Dropout mechanism, our work explores the problem of regularizing over-parameterization in neural networks from an evolutionary computing perspective. In addition, our work is also related to automated data augmentation [3, 17, 18, 35, 38]. Unlike most data augmentation methods that are usually applied specifically to the type of input data, our method works on the high-level representations of neural networks. It employs a more general design philosophy, and thus the same mechanism can be easily applied to different data types and tasks.

Our work is inspired by the parent selection methods [1, 6, 10, 14, 16, 22] in evolutionary computing. More specifically, our method is related to the Implicit Fitness Sharing [22] and Lexicase selection [1, 10, 16], in which hard cases are either weighted more heavily in the attention layers or required to be correctly predicted by some model variants in every generation, when the training samples are ordered in random sequences. The proposed ANS framework is designed to put selection pressure to guide the neural networks to use the right amount of neurons depending on model performance. Since the neural networks usually require batched training samples to work with large-scale datasets, we follow the general idea in [1] to make the selection framework suitable to be trained with batched samples.

We also take advantage of the attention mechanism, which has been proved to be useful in improving neural network performance with different architectural designs [4, 12, 34] in the context of deep learning. However, most of these methods rely on gradient-based training of the attention layers, in which case the updates of weights in the attention layers are correlated with the updates of weights in the neural network. This will result in co-adaptation of weights in both the attention layers and other layers in the neural network, which may still cause overfitting since the network can still learn to memorize all the training samples. On the other hand, our work evolves the self-attention module based on a combination of the proposed adaptive regularization method and gradients from the model prediction loss. In this way, we can prevent the co-adaptation of attention and neural network weights, and thus have a stronger regularization effect on the network.

Our work is also closely-connected to prior research on neural evolution [23, 28, 29, 32, 33], and neural architecture search [2, 19–21, 26]. The proposed ANS framework assumes a fixed neural network architecture and evolves different model variants to handle different input cases, which is different from the general neural evolution and architecture search methods that aim to evolve the network architectures. Our method can be further combined with neural evolution methods to co-evolve network variants and network architectures at the same time.

3 METHODS

In this section, we introduce the Adaptive Neural Selection (ANS) framework. ANS aims to evolve the behavior of selecting certain neurons from the deep neural networks to perform the prediction task based on the input training samples. The framework consists of two parts: a self-attention module and an adaptive regularization mechanism. An illustration of our method comparing to ordinary neural networks and the Dropout [31] is shown in Fig. 1.

3.1 Ordinary Neural Network

Consider a neural network with $c$ fully connected layers. Let $l \in \{1, \ldots, c\}$ denote the index of hidden layers. Let $x^{(l)}$ denote the input vector to layer $l$, and $y^{(l)}$ denote the output vector from layer $l$ before activation. $W^{(l)}$ and $b^{(l)}$ are the weight matrix and bias vector at layer $l$. The forward pass operation of an ordinary neural network at layer $l$ can be described as

$$
g^{(l)} = W^{(l)} x^{(l)} + b^{(l)}
$$

$$
x^{(l+1)} = f(y^{(l)})
$$

where $f(\cdot)$ is the activation function, such as the ReLU function $f(x) = \max(0, x)$.

The neural network is usually trained using back-propagation and gradient descent. We use $L_{\text{grad}}$ to denote the common gradient-based loss functions. For example, the classification image task usually use cross-entropy loss on the one-hot encoded output, described as

$$
L_{\text{grad}} = - \sum_{Y \in Z} (Y \cdot \log \hat{Y})
$$

$$
\hat{Y} = f(y^{(c)})
$$

where $Y$ is the one-hot encoded ground truth label in the set $Z$ of all the training labels, and $\hat{Y}$ is the corresponding network’s prediction. The prediction is usually calculated using the softmax function as $f$ on the last layer’s output.

For neural networks that have specific layers for feature extraction, such as convolutional neural networks (ConvNets), we also use the above formulation for the fully-connected layers in the network, which usually comes after the feature extraction layers.
3.2 Self-attention Module

To add the self-attention module, we use $z^{(l)}$ to denote an attention layer with another pair of weight matrix $W^a_{a}^{(l)}$ and bias vector $b^a_{a}^{(l)}$. The forward pass operation of a neural network with attention module can be described as

$$y^{(l)} = W^l x^{(l)} + b^{(l)}$$  \hspace{1cm} (5)

$$z^{(l)} = W^a_{a}^{(l)} f(y^{(l)}) + b^a_{a}^{(l)}$$  \hspace{1cm} (6)

$$x^{(l+1)} = g(z^{(l)}) f(y^{(l)})$$  \hspace{1cm} (7)

where $f(\cdot)$ is the activation function and $g(\cdot)$ is the gating function on the attention weights. In this work, we use the soft attention mechanism which uses the sigmoid function $g(x) = 1/(1 + e^{-x})$.

By adding the self-attention module, the neuron activations $f(y^{(l)})$ are now regularized by the attention units $g(z^{(l)})$. Since we have $g(z^{(l)}) \in (0, 1)$ for the sigmoid function, the neurons become selective according to the weights comparing to the ordinary neural network. We can also represent the ordinary neural network with this formulation by having $g(z^{(l)}) = 1$ for every neuron, and Dropout can be viewed as having random binary values of $g(z^{(l)})$. Thus, the self-attention module can achieve a larger space of sub-network structures comparing to Dropout.

While the weight matrix $W^a_{a}^{(l)}$ and bias vector $b^a_{a}^{(l)}$ for the attention layer can be trained in parallel through normal gradient descent and back-propagation, the resulting selection of neurons may not work well as a regularization for the neural network. As the self-attention module is a fully connected layer extended from the neural network, it may co-adapt with the neural network weight and thus result in overfitting. To solve this issue, we further introduce an adaptive regularization mechanism for the self-attention module, as describe in the next subsection.

3.3 Adaptive Regularization for Neural Selection

In the context of modern deep neural networks, with similar architectures and training protocols, better performance is usually achieved by network variants with deeper structures and parameters. However, the overfitting problem is also more likely to occur especially when training large neural networks with insufficient data. One thing that people usually do not know in advance and thus require lots of experiments and tuning is how many parameters works the best on the given dataset, that will not cause overfitting. A common way to resolve this issue is to have regularization on the neural network, and penalize it for having or relying on too many parameters. For example, Dropout forces the network to only use a random number of neurons, i.e., a sub-network, for prediction during training, and Weight Decay penalizes complexity by adding all the parameters to the loss function.

Most of these methods apply equally to all the training and testing samples, assuming that all the input samples follow the same distribution, and the neural network is trained to work with that distribution. However, some input samples have higher complexity, and thus may need more neurons to form a good representation. To explore this regime, we propose an adaptive regularization mechanism. For layer $l$ in the neural network, we use $g(z^{(l)})$ to denote the self-attention units. The regularization is calculated as

$$L_{reg} = \gamma \cdot \frac{1}{k} \| g(z^{(l)}) \|_1$$  \hspace{1cm} (8)

where $\gamma$ is a variable that controls the extent of regularization and $k$ is the number of all the neurons as a normalization factor.

We also introduce a strategy to calculate $\gamma$ depending on the model performance on current input samples. The idea is that for better training performance on a batch of data, the chance of overfitting is higher, and we thus need greater regularization to guide the network to use fewer neurons that may form more generalizable representations. To achieve this, we calculate $\gamma$ as

$$\gamma = \alpha \cdot M^\beta$$  \hspace{1cm} (9)

where $\alpha$ and $\beta$ are hyperparameters controlling the scale and variance of $\gamma$. $M$ denotes a non-negative metric of model performance on current input samples. In the context of image classification, for example, we use batch accuracy as the metric where $M \in [0, 1]$. With this formulation, we have $\lambda$ becomes larger when the model performance becomes better, and thus enforcing greater regularization on the neural networks.

3.4 Evolving Adaptive Neural Selection

Here we introduce the Adaptive Neural Selection (ANS) framework that combines the self-attention module and the adaptive regularization method. Inspired by parent selection methods in genetic programming, the ANS framework introduces a selection pressure to the current neural network by injecting regularization on the number of neurons currently being used for the input training sample. By putting the attention weights on a set of neurons for each training sample, the selection actually evolves different sub-network variants adaptively, and such evolution improves as the training process proceeds. The fitness of neuron selection is evaluated by the current model performance, and the way we optimize the neural selection is to select as few neurons as possible depending on the difficulty of predicting the input sample, in order to prevent overfitting on trivial cases or underfitting on hard ones. The full training procedure is described in Algorithm 1.

During the procedure of evolution, the framework trains the neural networks by using a combination of error gradient and regularization. With the help of gradient-based learning, the neural selection can be efficiently optimized and quickly reach convergence. In addition, since most neuroevolutionary methods tends to use non-gradient methods for optimization, such as Gaussian mutation, our framework can be easily extended to apply those techniques as well, by using the $L_{reg}$ term for fitness evaluation. However, in order to show the effectiveness of the proposed framework, we choose to not use those non-gradient optimization methods to ensure fair comparison to the ordinary gradient-trained models.

4 EXPERIMENTS

In this section, we implement and test the proposed ANS framework to common ConvNet architectures for the supervised image classification task. We compare our method against the Dropout method with different parameter settings. We also perform ablation study on the effect of hyperparameters of ANS.
We use similar training configurations that are commonly adopted. We use the CIFAR-10 and CIFAR-100 datasets [15] for the experiments. We use the ResNet-50 [9] and VGG-16 [30] models for the experiments. The initial learning rate is \(0.1\) at epoch 1 with weight decay of \(0.0001\). We decrease the learning rate by a factor of \(0.1\) at every epoch. The optimization method is stochastic gradient descent with Nesterov momentum of 0.9, with weight decay of \(1e-4\). The initial learning rate is \(0.1\) for ResNet-50, and \(0.01\) for VGG-16, given the fact that VGG-16 has more parameters and thus needs a smaller learning rate to prevent divergence. We decrease the learning rate by a factor of \(0.1\) at epoch 60 and 90 for better convergence. All the models are trained from scratch with standard initialization methods as in the original work. We also follow the common data augmentation pipeline in [9], which is random cropping and horizontal flipping. All the training jobs are implemented with PyTorch [25] library and performed on cluster nodes with a single GPU. The test results are obtained on predicting with the single image only, without ensembling.

### 4.3 Experiment Configuration

We use similar training configurations that are commonly adopted in prior works [5, 9]. For all the experiments, we use a batch size of 64 and a total number of epochs of 120. The optimization method is stochastic gradient descent with Nesterov momentum of 0.9, with weight decay of \(1e-4\). The initial learning rate is \(0.1\) for ResNet-50, and \(0.01\) for VGG-16, given the fact that VGG-16 has more parameters and thus needs a smaller learning rate to prevent divergence. We decrease the learning rate by a factor of \(0.1\) at epoch 60 and 90 for better convergence. All the models are trained from scratch with standard initialization methods as in the original work. We also follow the common data augmentation pipeline in [9], which is random cropping and horizontal flipping. All the training jobs are implemented with PyTorch [25] library and performed on cluster nodes with a single GPU. The test results are obtained on predicting with the single image only, without ensembling.

### 4.4 Image Classification Results

We apply the ANS framework on ResNet-50 and VGG-16. For comparison, we also implement the baseline method of the vanilla architectures and add Dropout at rate 0.3 and 0.5. Note that the original implementation of VGG-16 has a default Dropout at 0.5, but here for the vanilla VGG-16 we remove the Dropout for fair comparison.

Table 1 shows the test result with ResNet-50 on CIFAR-10 and CIFAR-100. Since the ResNet-50 architecture does not have an intermediate fully connected layer between the feature pooling layer and the classification layer, both Dropout and ANS are applied only on the features layer after average pooling. We can observe that Dropout does not show positive effect on the model performance. However, our ANS method significantly improves the model performance, especially on the harder benchmark CIFAR-100.

For VGG-16, the results are shown in Table 2. Given the VGG-16 architecture, we apply the Dropout and ANS on the last two fully connected layers before the classification layer. The implementation with Dropout rate at 0.5 is identical to the original VGG-16 model. We can first observe that Dropout significantly improves the VGG-16 model, because VGG-16 has more parameters and connection that may be easier to cause overfitting. The proposed ANS method further improves the model performance, outperforming the Dropout method.

One of the drawbacks of methods such as Dropout and its variants is they require specific design and tuning to work with different architectures. For example, [37] shows that dropping neurons everywhere is not as good as only dropping the neurons in the vertical
connections for a multi-layered LSTM network [11]. Similarly, our results show that even for similar ConvNet architectures, the application of Dropout does not always benefit the model. However, our method consistently improves the neural network despite the underlying architectures and datasets.

4.5 Training Analysis

In Fig. 2, we visualize the training process of the experiments, comparing our method to the vanilla model and Dropout. For ResNet-50, we can observe that with Dropout, the model has similar or slower convergence than the vanilla model. However, our method achieves superior convergence. Since for ResNet-50 the ANS method is directly applied on the final feature representation layer after the pooling operation, it is able to improve the learning process by putting more effort on the difficult cases. This is because the selection pressure limits the usage of neurons for easier cases, and thus the loss on difficult cases has larger weight on the network updates.

For the VGG-16 model, while we can still observe that the convergence of ANS is slightly better than Dropout, the vanilla model actually converges faster. Considering the fact that the vanilla VGG-16 has significantly worse testing performance than using Dropout and ANS (as shown in Table 2), we can see that the vanilla VGG-16 easily overfits the training data if no regularization method is used. This is because VGG-16 has many more parameters within the last two fully connected layers. Regarding the complexity of the VGG-16 model, while the convergence speed is similar, ANS improves the generalization capability of VGG-16 with little cost on the training process.

In addition, since CIFAR-10 has fewer classes and more data for each class, it is usually easier to work with than CIFAR-100. Most of the analysis and results are better illustrated on CIFAR-100.
4.6 Ablation Study

To further validate the effectiveness of the proposed ANS method, we perform ablation study on the components and hyperparameters of ANS. The experiment settings are identical to the experiments in previous sections, where we test ANS with ResNet-50 and VGG-16 on both CIFAR-10 and CIFAR-100.

4.6.1 Effectiveness of Components. The proposed ANS framework consists of two components: the self-attention module and the adaptive regularization loss. In this ablation study, we validate the effectiveness of each component by having the test setting that removes the adaptive regularization loss by letting $\alpha = 0$, meaning the self-attention module is trained only using gradients from the classification loss, without the adaptive regularization. The results are shown in Table 3 and Table 4.

We can first observe that with the self-attention module only, ANS is able to improve the model performance by an obvious margin. Similar results have been shown in some recent works [12, 34] that utilize attention-like mechanism in tuning deep neural network architectures.
Secondly, by adding the adaptive regularization, the performance is further improved to a larger extent. For example, the testing accuracy is boosted by 1.08% by adding adaptive regularization to the self-attention-only ResNet-50, while the self-attention itself adds 0.35% to the vanilla model. The results shows that the adaptive regularization mechanism is able to evolve better neural selections comparing to just using end-to-end gradient training.

4.6.2 Hyperparameters. The fitness function of neural selection $\gamma$ is controlled by two hyperparameters: $\alpha$ and $\beta$, as stated in Eq. 9. We investigate how different hyperparameter settings may influence the model performance with ANS, as the selection pressure is tuned by changing them. Fig. 3 shows the testing results on different $\alpha$ and $\beta$ settings in the format of heatmaps with the exact accuracy number in each cell. In order to properly weigh the two losses for joint learning, we limit the scale of searching space of $\alpha$ and $\beta$ by having $\alpha \in \{0.5, 1, 2\}$ and $\beta \in \{0.5, 1, 2\}$. We test for every combination of the two hyperparameters within this space.

In general, we can see that the framework is relatively robust to different hyperparameters settings. For example, for the ResNet-50 model on CIFAR-100, the worst-performing hyperparameter setting ($\alpha = 2$, $\beta = 0.5$) has testing accuracy 0.7591, which is still higher than using Dropout($\rho = 0.3$) which has accuracy 0.7587.

While there is no obvious pattern and correlation in terms of the hyperparameters, it should be noted that the hyperparameters of ANS can be problem dependent, just like hyperparameters for other selection methods in evolutionary computing (such as the tournament size parameter for tournament selection). However, we found that a setting of $\alpha = 1$ and $\beta = 1$ has been robust for most of the cases.

5 CONCLUSION AND FUTURE WORK

In this paper, we propose the Adaptive Neural Selection (ANS) method and a framework for deep neural networks to evolve the behavior of selecting specific neurons from the networks to perform the prediction task adaptively based on the current input data. ANS can significantly improve the model performance on generalization to unseen test cases without slowing down the training process. Ablation study also shows that ANS has robust performance over different hyperparameter settings.

While this work only applies ANS on fully-connected layers, ANS can be easily extended to other network architectures, such as convolutional layers, by transforming it to variants with specific structures. ANS can also be optimized by using non-gradient neuroevolutionary techniques, which may further improve the evolution of its weights.

In addition, while we keep the basic network architecture unchanged and only evolve the selection of neurons, the ANS framework can also be used to evolve the network architectures, serving as a strategy for neural architecture search. For example, instead of putting regularization on attention weights, we can alternatively use ANS to regularize the complexity of the network architecture by removing layers, connections, etc. We look forward to a deeper analysis on the effectiveness of combining ANS with other neural network evolution strategies.

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