Evolving Deep Neural Networks

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Abstract

Genetic algorithms have long been successfully applied to optimize the weights of neural networks. The genetic concept of crossover, recombining components to form a stronger one, applies well to DNNs. This paper elaborates on the performances of two automated evolutionary methods for optimizing deep learning architectures on the relevant and important tasks of language modeling and image classification. The first of these methods is based on a hierarchical genetic representation scheme, and the second is based on evolving populations of chromosomes and crossing over the strongest amongst them. Presented are the implementations of these algorithms for both tasks as well as results on the CIFAR-10 dataset, demonstrating classification quality comparable to that of literature and setting the stage for the future work of merging these methodologies.

1 Introduction

With the advent of big data and superior hardware, scaling very powerful machine learning systems has become more realistic than ever before. Thus, there has recently been an influx of advances in training Deep Neural Networks (DNNs), specifically Convolutional Neural Networks and Recurrent Neural Networks, to tackle a multitude of problems in computer vision, language processing, and many other domains.

A challenge of widespread adaption of DNNs is that the most successful networks are the ones that often are the most complex, with extremely intricate topologies to sort through and hundreds of hyperparameters to optimize. Given the difficulty of the task, alternative methods of identifying network architectures and optimizing the hyperparameters have been sought after. Such methods are thought of as preferable over relying on human engineers to make the precise design choices necessary to build the strongest networks. One alternative method would be for the human engineer do the high-level organizational work, and for the computer do the bulk of the work on identifying an optimal network architecture.

This paper demonstrates the success of two evolutionary algorithms on choosing optimal network architectures for evolving LSTMs for the task of language modeling and CNNs for the task of image classification. We demonstrate algorithms that utilize hierarchical genetic representation schemes and incremental increased topology complexities to evolve networks comparable to the existing literature.

2 Background

The field of neuroevolution, which refers to applying Evolutionary Algorithms to evolving neural networks, emerged in the 90's as a way of creating neural networks prior to the rise of GPU-driven supervised learning. Methods were developed such as SANE, [4] which evolved the synaptic weights of the network, while another class of methods was developed to evolve the structures of the neural networks. While the former has

largely been overshadowed by the achievements of backpropagation and gradient descent, the latter lives on thanks to the development of Neuroevolution of Augmenting Topologies (NEAT) [7]. As further discoveries like ReLU activation functions and batch normalization as well as advances in GPU design allowed the construction of deeper and larger neural networks, a new field of "meta-learning" emerged. Meta-learning utilizes learning techniques to optimize the hyperparameters of deep neural networks (DNNs), generally either using convolutional layers for image classification task or LSTMs for language modeling tasks. Recent work has shown impressive results in the field of meta-learning on benchmark datasets with Bayesian Optimization [6], Reinforcement Learning [8], and Evolutionary Algorithms [5]. CoDeepNEAT is an algorithm developed recently by Mikkulainen et. al. which marries the fields of neuro-evolution and meta-learning [3]. CoDeepNEAT is an extension of NEAT to DNNs. Each node gene in the chromosome is no longer a single neuron but is now treated as an entire layer in a DNN with hyperparameters determining the type of layer (recurrent, dense, etc.) and that layer's properties. The chromosome also tracks the connections between layers, although these connections are no longer evolved as gene's and their weights are determined through supervised learning. Each chromosome is evaluated by being compiled into a network, trained for a fixed number of epochs, and assigned a fitness equal to it's validation accuracy.

The macro-view of the CoDeepNEAT algorithm involves two main components: modules and blueprints. Blueprint chromosomes are made up of genes representing a linearly connected set of modules. Module chromosomes are made up of genes representing an interconnected set of DNN layers. The key innovation of CoDeepNEAT is that these two interconnected components are represented as separate populations which are evolved in parallel. The fitnesses of the modules are determined stochastically from the fitnesses of the blueprints of which they are a part. One key aspect of CoDeepNEAT the is largely unaddressed within the paper is the structure of the software implementations of the blueprints and modules. The authors, in fact, did not settle on a single implementation; instead, they came up with distinct implementations for each different benchmark test that CoDeepNEAT was demonstrated on.

Thankfully, recent research [1] tackles this exact problem. One particular study focuses on developing a hierarchical representation of DNNs, specifically deep convolutional neural networks. The core concept of this representation is that at every potential hierarchical level, a DNN can be represented as a directed acyclic graph where each node is a tensor (or "feature map") and each edge represents some nonlinear operation. At the lowest level, these operations are considered to be neural network layers, in this case drawn from a fixed list of convolutional layers considered to be "primitive operations." The key insight behind this fixed list is that a wider variation of layers can be created from an arrangement of simple fixed layers. For example, two parallel convolutional layers with 16 filters each is exactly equivalent to a single convolutional layer with 32 filters. The authors of this paper demonstrate the usefulness of this representation on image classification benchmarks using both a random search and a simple evolutionary scheme.

3 Implementation

3.1 CoDeepNEAT

Our implementation of CoDeepNEAT is based largely on the given description of the application of CoDeepNEAT to language modeling with the PTB and to image classification with CIFAR-10. We wrote our implementation in Python3.5 on top of both the NEAT3 code used in class and the Keras deep learning API

with a TensorFlow backend. Keras is a widely used and user-friendly API that supports a range of backend tensor operation libraries, thus allowing our implementation to be highly portable. The code describing the Populations and Species from NEAT3 was largely preserved in our implementation, as these components function nearly identically in CoDeepNEAT as they do in NEAT. Two major changes were introduced: an entirely new encoding scheme for the chromosomes and genes was introduced, and the evolution routine itself was modified to support coevolution. The relationship between the encodings of the blueprint and module chromosomes is shown below in Figure 1.

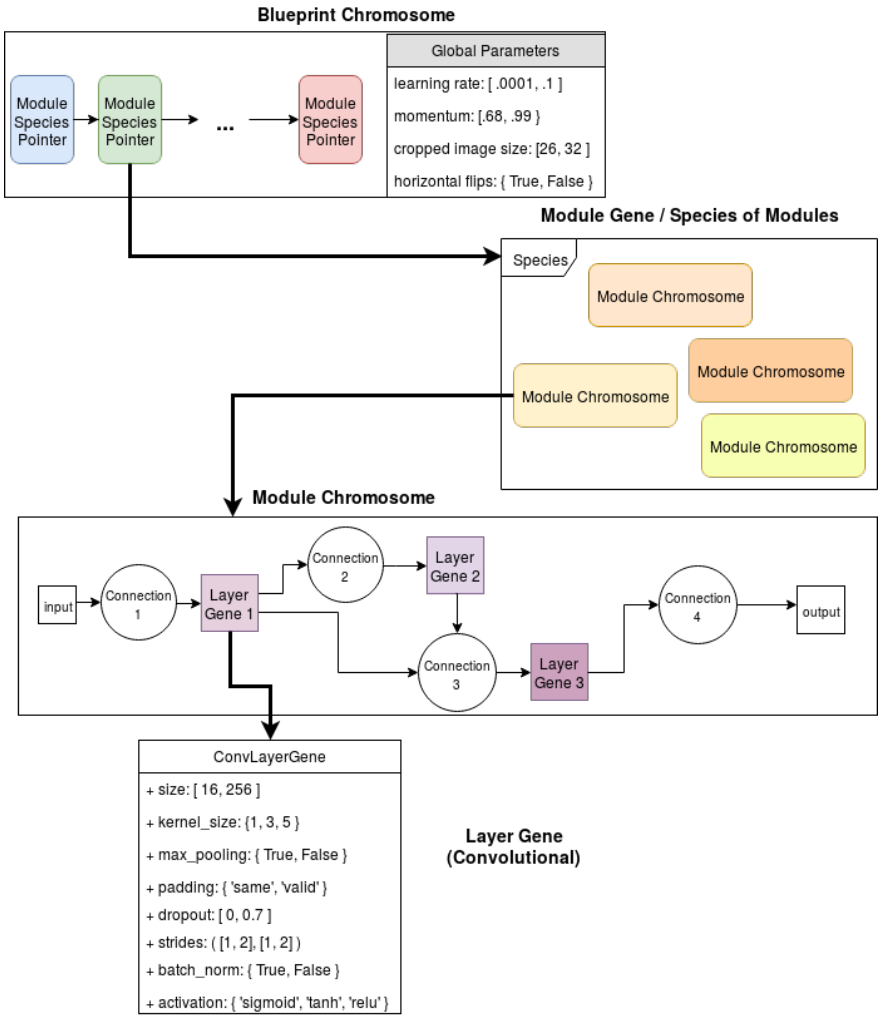


Figure 1: Design of CoDeepNEAT chromosomes and genes

Each blueprint chromosome contains both an ordered list of module genes and a dictionary of global hyper-parameters. Each of the module genes is actually a pointer to a species of module chromosomes, which must be checked after each time the module population is speciated to avoid pointing to a nonexistent species. When a blueprint is compiled into a network a representative module for each species referred to in its genome is sampled from a uniform distribution over the species. This means that two module genes point-

ing to the same module species will be replaced with the same module every time a network is generated, but the identity of that module can vary for every new network. The blueprint chromosome includes two forms of mutations: inserting a new module gene at a random index and randomly reassigning the pointer of a module gene.

Each module chromosome tracks a set of layer genes and the connections between each of those genes. Our module chromosome supports two forms of mutation: adding a layer gene between two randomly chosen points and mutating individual layer genes. The connections are shown as nodes in the graph given in Figure 1 but in practice encode both the edges of that graph and the merging of tensors that must be performed for any layer receiving more than one input. Our chosen merge method was to concatenate along the last dimension, which is equal to number of filters for convolutional layers and the output for recurrent and dense layers. Convolutional layers also are downsampled via max pooling to the smallest of the spatial dimensions in the merge. The layer genes encode a either a Conv2D, LSTM, or Dense Keras layer, storing the the parameters for that layer in a dictionary. Figure 1 shows the available range of parameter settings, but each individual layer gene's dictionary actually stores the value used for that layer. These parameters can all be modified through mutation.

CoDeepNEAT(*maxGenerations*, *numNetworks*, *data*)

```
1  INITIALIZE(modulePopulation)          // as randomly parametrized simple modules, speciate
2  INITIALIZE(blueprintPopulation)       // as random small blueprints, speciate
3  generation = 0
4  while generation < maxGenerations
5      for i = 0 to numNetworks
6          bp = RANDOM SAMPLE(blueprintPopulation)
7          model = ASSEMBLE(bp)
8          accuracy = FIT(model, data)
9          bp.fitness = bp.fitness + accuracy
10         bp.numUse = bp.numUse + 1
11         for module in bp
12             module.fitness = module.fitness + accuracy
13             module.numUse = module.numUse + 1
14     for indiv in blueprintPopulation + modulePopulation
15         module.fitness = module.fitness ÷ module.numUse
16     mparents = TOURNAMENT SELECT(allModuleSpecies)
17     mchildren = REPRODUCE(mparents)       // includes crossover and mutation
18     modulePopulation = mchildren
19     SPECIATE(modulePopulation)
20     bparents = TOURNAMENT SELECT(allBlueprintSpecies)
21     mbchildren = REPRODUCE(bparents)      // includes crossover and mutation
22     blueprintPopulation = bchildren
23     SPECIATE(blueprintPopulation)
24     generation = generation + 1
```

The above pseudocode shows the changes made to NEAT to support coevolution. Two populations are now tracked instead of one. The populations are involved in parallel, analogous to how evolution works in NEAT,

except the module population must be updated first to avoid invalid module species pointers and the fitnesses are assigned to the each individual probabilistically from the fitnesses of a number of generated networks. Our estimator for the fitness metric of each blueprint and module sets the fitness as the average fitness of the networks that a particular blueprint or module was used in. Unused individuals are given fitness .01 higher than that of the population average in order to encourage using them down the road.

3.2 Hierarchical Representation

Our implementation of the hierarchical representation of neural networks was also written in Python3.5 on top of Keras. The representation consists entirely of Motifs, which encode a directed acyclic graph. Each Motif maintains an adjacency matrix containing the index of each of the operations represented as the edges between the nodes in the graph (which represent tensors). Operations for a level 2 Motif are pre-defined primitives. Operations at higher levels are a set of Motifs at the previous level. We defined two types of architectures, a Flat architecture which contains a single level 2 Motif (in our experiments this has 11 nodes) and a Hierarchical Architecture which contains a single top level Motif and a set number of lower level motifs (in our experiments this was a level 3 Motif with 5 nodes and 6 level 2 Motifs with 4 nodes each).

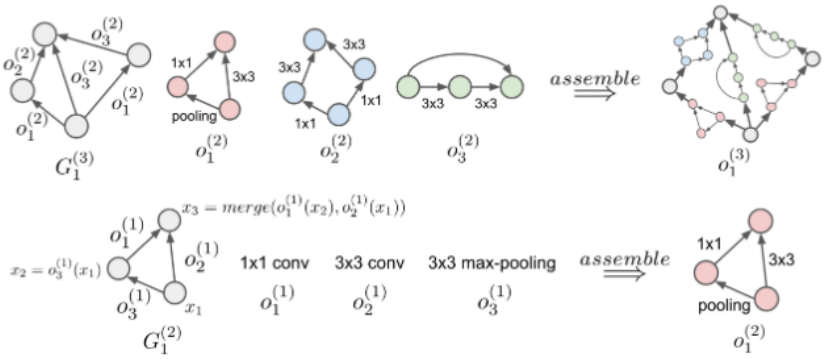


Figure 2: Hierarchical representation of onvolutional network

The above Figure 2 shows the assembly of a level 2 Motif (bottom) and level 3 Motif (top). Merging was assigned as last-dimension concatenation, which did not require down-sampling as all operations within Motifs are padded to preserve spatial dimensions in convolutional networks. In order to be used, the architectures we defined were used as cells in the generic architectures shown in Figure 3. Mutation on an architecture involved sampling a random level (¿1) over uniform probability, then sampling a random Motif at that level over uniform probability, then sampling a random successor node in the Motif over uniform probability, then sampling a random predecessor node in the Motif over uniform probability. The operation between these two nodes was reassigned randomly from the list of available operations over a uniform probability distribution.

4 Experiments

In order to examine the performance and adaptiveness of our implementation, we performed experiments on both image classification and language modeling benchmark datasets. In the following subsections, the

benchmark datasets are briefly introduced and the experimental setup for both CoDeepNEAT and Hierarchical Representation implementations are documented.

4.1 Image Classification

In our image classification experiments, we used CIFAR-10 dataset as the dataset. The CIFAR-10 dataset contains colored 32*32 images (3 channels) in 10 different categories. It has 50,000 images in the training set and 10,000 images in the testing set.

4.1.1 CoDeepNEAT

For our CoDeepNEAT experiment, we evolved the topology of a CNN to maximize its classification performance on the CIFAR-10 dataset. We initialized the blueprint population with size of 15 and the module population with size of 10. From those two populations, 25 CNNs were assembled for fitness evaluation in every generation. During fitness evaluation, the training set was divided into a 42,500 image training subset and 7,500 image validation subset so that the testing dataset was unseen to the evolution process. Given that training deep neural networks could be computationally expensive and our limited resources, each model was trained for 8 epochs using the default Adam optimizer. The data augmentation included horizontal and vertical shifts with a factor of 0.1 and random horizontal flips of the images. After training, the validation subset was used to determine the fitness of the models. After the evolution, the best performing models of each generation was trained on the entire training set (50,000 images) and evaluated on the test set (10,000 images). Table 1 shows that the parameter settings used in the experiments. Table 2 shows the layer parameters that could be mutated during mutation.

Parameter	**Setting**
Generations	25
Module Population	10
Blueprint Population	15
Model Population	25
Input nodes	32, 32, 3
Output nodes	10
Prob. to add Conv. layer	1.0
Prob. to add layer	0.1
Prob. to mutate layer	0.3
Prob. to add module	0.05
Prob. to switch module	0.1
Elitism	1

Table 1: CoDeepNEAT parameter settings used in the experiments.

4.1.2 Hierarchical Representation

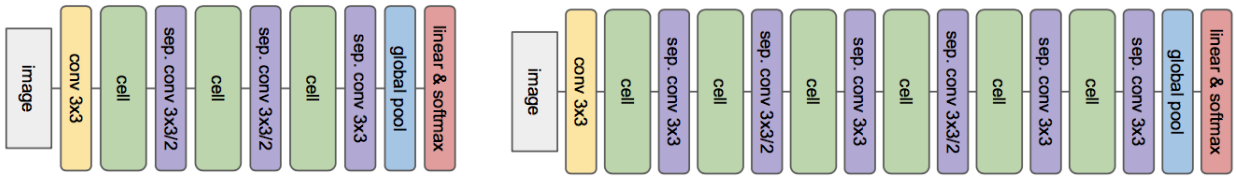
For our Hierarchical Representation experiment, we performed both evolutionary search and random generation of the architecture.

Conv. Parameter	Range
Number of Filters	[16, 256]
Max Pooling	{True, False}
Kernel Size	{True, False}
Dropout Rate	[0, 0.7]
Dense Parameter	**Range**
Output nodes	[16, 256]
Dropout Rate	[0, 0.7]

Table 2: layer parameters available for mutation.

For the evolutionary search, we randomly generated 50 modules using the hierarchical representation. Then we performed 100 mutations on each generated modules to obtain the initial population. In order to evaluate as many models as possible, we used a small model showed in Fig. 3a for fitness computation. Each module in the initial population was inserted into the small model and trained on a training subset of 40,000 images. For data augmentation, each training image was randomly cropped to 24*24 and randomly horizontally flipped. The fitness of each module was evaluated on the 10,000 image validation dataset. After evaluating the fitnesses of the initial population, 5% of the population would be randomly picked and the module with the highest fitness in the 5% would go through a mutation. The mutated module would be evaluated and added to the population. We set the evolution to have 150 steps so the final population size was 200. After the evolution, the module with the highest fitness overall was inserted into a large model showed in Fig. 3b. The model was trained with the entire training set and evaluated on the test set.

For the random generation, we randomly generated an architecture using the hierarchical representation, and performed 100 mutations on the initial architecture. Then the mutated architecture was inserted into the large model. The model was trained with the entire training set and evaluated on the test set.



(a) small model

(b) large model

Figure 3: Two models used for CIFAR-10 [1]

4.2 Language Modeling

Language modeling is a fundamental task in artificial intelligence. A language model simply is a probability distribution over a sequence of words or characters and is used to predict the next word in the sequence. We modeled the Penn Tree Bank (PTB) dataset, a widely used corpus with 10000 training words in its vocabulary. The training set contains 929,000 words, the validation set 73,000 words, and the test set

contains 82,000 words [2].

4.2.1 Evaluating Language Models

Let us denote a given sequence of n words in the training corpus to be

$$w_1 : n$$

. Training the LSTM involves minimizing the negative log-likelihood of the sequence

$$NLL = -\sum_{n=1}^{N} logP(w_n|w_{1:n-1})$$

. The Perplexity of the model of the sequence, given below, is calculated over the test set. [2]

$$PPL = exp(NLL/T)$$

4.2.2 CoDeepNEAT

For the sole CoDeepNEAT run on the PTB, We evolved the topology of a CNN to maximize its perplexity on the PTB test set. We initialized the blueprint population with size of 15 and the module population with size of 10. The PTB validation set was used for fitness evaluation, allowing for saving the test set. Given that training deep neural networks could be computationally expensive and our limited resources, each model was trained for 3 epochs using the default Adam optimizer. After the evolution, the best performing models of each generation was trained on the entire training set and evaluated on the PTB test set.

4.2.3 Hierarchical Search

For the sole evolutionary search conducted on the language modeling task, we randomly generated 10 modules using the hierarchical representation. Then we performed 20 mutations on each generated modules to obtain the initial population. LSTM variants of the small model seen in Figure 1a are representative of the generated modules. Analogous to the process for Image Classification, each module in the initial population was inserted into the small model and trained on PTB training set. The fitness of each module was then evaluated on the validation set. After evaluating the fitnesses of the initial population, 5% of the population would be randomly picked and the module with the highest fitness in the 5% would go through a mutation. The mutated module would be evaluated and added to the population. After 50 steps of evolution, the module with the highest fitness overall was inserted into a large model, which in turn was trained with the entire training set and will be evaluated on the test set.

5 Results

5.1 Language Modeling

Despite our confidence in the evolutionary algorithms presented in this work, the ability of those algorithms to produce literature-comparable language modeling results necessitates both profound computational power and time, both of which we did not have at our disposal at a large enough degree to complete the sole run of

LSTM Parameters	Fixed
Max Sequence Length	35
Batch Size	20
Output nodes	49
Loss	Sparse Categorical Entropy

Table 3: Fixed parameters for Language Modeling for both Hierarchical Search and CoDeepNEAT

each algoritm on the PTB. Thus, no conclusive results for the language modeling task are presented at this time.

5.2 Image Classification

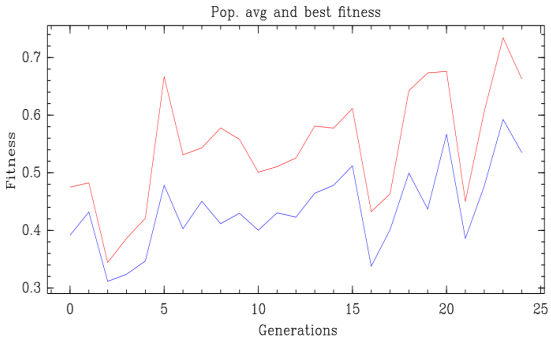
We introduce the results for both CoDeepNEAT and Hierarchical Search, and compare the two algorithms in terms of performance and computational complexity.

5.2.1 CoDeepNEAT

The best network for CoDeepNEAT was found in the 24th generations, as shown in Figure 4. The network reached 86.33% of test accuracy after 50 epochs of training.

Figure 4: The test accuracies of the best models across generations

(a) Blueprint fitness



(b) Module fitness

Figure 5: Average and highest fitness of Blueprint and Module populations across generations

5.2.2 Hierarchical Search

We noticed that the flat representation would produce much larger networks than hierarchical representation, as shown in Table 4 and we did not have the resources to fully evaluate the best performing network from the flat representation experiment.

Experiment	**Avg. Fitness**	**Parameters(m)**
Flat Representation, random search (50 samples)	0.7347 ± 0.0464	1.059 ± 0.550
Hier. Representation, random search (50 samples)	0.6303 ± 0.0940	0.246 ± 0.137
Hier. Representation, evolution steps (200 steps)	0.6508 ± 0.0691	0.337 ± 0.160

Table 4: Average results from each experiment

Best model	**Test Accuracy**	**Parameters(m)**
CoDeepNEAT	0.8633	18127642
Hier. Representation, random sampling	0.8535	665546
Hier. Representation, random search (50 samples)	0.8927	651594
Hier. Representation, evolution steps (200 steps)	0.8943	1173578

Table 5: Best performing models from each experiment

6 Discussion

The results of this paper show that both hierarchical and multi-layered evolutionary approaches to optimizing DNNs is both feasible and develops DNNs comparable to those with hand-designed architectures. We demonstrate results comparable to benchmark models on the CIFAR-10 image classification dataset and present a ready-to-go platform for evolving LSTMs to tackle language modeling. The potential of our work is still largely untapped due to the enormous computational power necessary to train the necessary number of

networks for obtaining the best network architectures through evolution. As more computational resources and time become more available to us, we expect to evolve novel network architectures while still achieving, at the very least, the benchmark scores on the PTB and CIFAR-10 datasets.

7 Ongoing and Future Work

The most immediate next goal of this work will be to evolve, using both CoDeepNEAT and the hierarchical representation algorithms, and test DNNs for the task of modeling the PTB. Initial (but incomplete) experimentation has been promising, with validation-perplexity in the range of approximately 150-220 when with just a few epochs of training through both methods. We aspire to improve upon the test-perplexity score of 78, the best score found in literature that was achieved on PTB with evolutionary algorithms [3]

Our ultimate goal is to create a single unified evolutionary framework capable of evolving a deep neural network optimally designed for any language modeling and image classification task. In order to do this, we've focused our effort on using evolution to search solely for high performing network topologies. Current work is focused on combining the hierarchical representation of neural networks with the multi-level evolution scheme of CoDeepNEAT to allow for simultaneous evolution on three different hierarchical levels.

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