Automatic model selection for neural networks

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***Abstract*—Neural networks and deep learning are changing the way that artificial intelligence is being done. Efficiently choosing a suitable model (including hyperparameters) for a specific problem is a time-consuming task. Choosing among the many different combinations of neural networks available gives rise to a staggering number of possible alternatives overall. Here we address this problem by proposing a fully automated framework for efficiently selecting a neural network model given a specific problem (whether it is classification or regression). Our proposal focuses on a distributed decision-making algorithm for keeping the most promising models among a pool of possible models for one of the major neural network architectures, Multi-Layer Perceptrons (MLPs). This work develops Automatic Model Selection (AMS), a modified micro genetic algorithm that automatically and efficiently finds the most suitable neural network model for a given dataset. Our contributions include: a simple list based encoding for neural networks as genotypes in an evolutionary algorithm, new crossover and mutation operators, the introduction of a fitness function that considers both, the accuracy of the model and its complexity and a method to measure the similarity between two neural networks. Our evaluation on two different datasets show that AMS effectively finds suitable neural network models while being efficient in terms of the computational burden, our results are compared against other state of the art methods such as Auto-Keras and AutoML.**

***Index Terms*—artificial neural networks, model selection, hyperparameter tuning, distributed computing, evolutionary algorithms.**

I. Introduction

MACHINE learning studies algorithms that improve themselves through experience. Given the large amounts of data currently available in many fields such as engineering, biomedical, finance, etc, and the increasingly computing power available machine learning is now practiced by people with very diverse backgrounds. Increasingly, users of machine learning tools are non-experts who require off-the-shelf solutions. Automated Machine Learning (AutoML) is the field of machine learning devoted to developing algorithms and solutions to enable people with limited machine learning background knowledge to use use machine learning models easily. Tools like WEKA [1], PyBrain [2] or MLLib [3] follow this paradigm. Nevertheless, the user still needs to make some choices which not may be obvious or intuitive (selecting a learning algorithm, hyperparameters, features, etc) thus leading to the selection of non optimal models.

Recently, deep learning models (CNN, RNN, Deep NN) have gained a lot of attention due their improved efficiency on complex learning problems and their flexibility and generality for solving a large number of problems such as: regression, classification, natural language processing, recommendation systems, etc. Furthermore, there are a lot software libraries which makes their implementation easier. TensorFlow [4], Keras [5], Caffe [6] and CNTK [7] are some examples of such libraries. Despite the availability of such libraries and tools, the task of picking the right neural network model and its hyperparameters is usually complex and iterative in nature specially among non computer scientist.

Usually, the process of selecting a suitable machine learning model for a particular problem is done in an iterative manner. First, an input dataset must be transformed from a domain specific format to features which are predictive of the field of interest, once features have been engineered users must pick a learning setting appropriate to their problem, e.g. regression, classification or recommendation. Next users must pick an appropriate model, such as support vector machines (SVM), logistic regression or any flavor of neural networks (NNs). Each model family has a number of hyperparameters, such as regularization degree, learning rate, number of neurons, etc, and each of these must be tuned to achieve optimal results. Finally, users must pick a software package that can train their model, configure one or more machines to execute the training and evaluate the model's quality. It can be challenging to make the right choice when faced with so many degrees of freedom, leaving many users to select a model based on intuition or randomness and/or leave hyperparameters set to default, this approach will usually yield suboptimal results.

This suggests a natural challenge for machine learning: given a dataset, to automatically and simultaneously chose a learning algorithm and set its hyperparameters to optimize performance. As mentioned in [1] the combined space of learning algorithm and hyperparemeters is very challenging to search: the response function is noisy and the space is high dimensional involving both, categorical and continuous choices and containing hierarchical dependencies (e.g. hyperparameters of the algorithm are only meaningful if that algorithm is chosen). Thus, identifying a high quality model is typically costly (in the sense that entails a lot of computational effort) and time consuming.

To address this challenges we propose Automatic Model Selection (AMS) a flexible and scalable method to automate the process of selecting artificial neural network models. The key contributions of this paper include: 1) a simple, list based encoding of neural networks as genotypes for evolutionary computation algorithms, 2) new crossover and mutation operators to generate valid neural networks models from an evolutionary algorithm, 3) the introduction of a fitness function that considers both, the accuracy of the model and its complexity and 3) a method for measuring the similarity between two neural networks. All these components together form a new method based on an evolutionary algorithm, which

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we call AMS, and that can be used to find an optimal neural network architecture for a given dataset.

The remainder of this paper is organized as follows: Section II formally introduces the model selection problem. The related work is briefly reviewed in Section III. The AMS algorithm and all of its components are described in detail in Section IV, experiments to test the algorithm and comparison against other state of the art methods are presented in Section V. Conclusions and future work are discussed in Section VI.

II. Problem Statement

In this section we mathematically define the general neural network architecture search problem. Consider a dataset $\mathcal{D}$ made up of training points $d_i = (\mathbf{x_i}, \mathbf{y_i}) \in \mathcal{X} \times \mathcal{Y}$ where $\mathcal{X}$ is the set of data points and $\mathcal{Y}$ is the set of labels. Furthermore, lets split the dataset into training set D_t, cross validation set D_v, and test set D_e. Given a neural network architecture search space $\mathcal{F}$ the performance of a neural network architecture $f \in \mathcal{F}$ on trained on $\mathcal{D}_t$ and validated with $\mathcal{D}_v$ is defined as:

$$p = Per(f(D_t); D_v), \tag{1}$$

where $Perf(.)$ can be any standard or custom cost metric, e.g. accuracy, precision, mean squared error, etc. Commonly used performance indicators can be found in Table XIV.

Finding a neural network $f^* \in \mathcal{F}$ that achieves a good performance has been explored in [8], [9] among others. While this task alone is challenging, usually the efficiency of f^* is not measured. Indeed, it turns out that there can be several candidate models that can attain similar performance with improved efficiency. By efficiency we mean, in practical terms, how fast is to train f^* as compared to other possible solutions.

In this paper we aim to achive neural network models f^* that not only exhibit good performance in $\mathcal{D}$ as measured by p but also achieves such performance using a simple structure, which directly translates to improved efficiency of the model. To measure the complexity of the architecture we make use of the number of trainable parameters $w(f)$ of the neural network, we will also refer to $w(f)$ as the "size" of the neural network.

The problem of finding an neural network f that achieves both a good performance on the dataset $\mathcal{D}$ with a simple model can be mathematically stated as the following multiobjective optimization problem:

$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \quad (p(f), w(f)) \tag{2}$$

In this paper we develop an algorithm to efficiently solve Eq. 2.

III. Related Work

Automated machine learning has been of research interest since the uprising of deep learning. This is no surprise since selecting an effective combination of algorithm and hyperparameter values is currently a challenging task requiring both deep machine learning knowledge and repeated trials. This is not only beyond the capability of layman users with limited computing expertise, but also often a non-trivial task even for machine learning experts [10].

Until recently most state-of-the-art image classifier architectures have been manually designed by human experts. To make the the process easier and faster, researchers have looked into automated methods. These methods' goal is to find, withind a pre-specified resource limit (usually specified in terms of time, number of algorithms and/or combintations of hyperparameter values), an effective algorithm and/or combination of hyperparameter values that maximize the accuracy measure on the given machine learning problem and data set. Using an automated machine learning, the machine learning practitioner can skip the manual and iterative process of selecting and efficient combination of of hyperparameter values and neural network model, which is labor intensive and requires a high skill set in machine learning.

In the context of deep learning , neural architecture search (NAS) which aims to search for the best neural network architecture for the given learning task and dataset, has become an effective computational tool in AutoML. Unfortunately, existing NAS algorithms are usually computationally expensive where its time complexity can easily scale to $O(nt)$ where n is the number of neural architectures evaluated, and t is the average time consumption for each of the n neural networks. Many NAS approaches such as deep reinforcement learning [11], [12], [13] and evolutionary algorithms [14], [15], [16], [17] require a large n to reach good performance. Other approaches include Bayesian Optimization [18], [19] and Sequential Model Based Optimization (SMBO) [20], [21], nevertheless often times this approaches are as expensive as NAS while being more limited as to what kind of models they can explore.

In the recent years a number of tools have been made available for users to automate the model selection and/or hyperparameter tuning, in the following we present a brief description of some of them that share similarities with out method and will serve as comparisson.

A. Auto-Keras

Write a brief description of the method here

B. AutoML Vision

Write a brief description of the method here

C. Auto-sklearn

Auto-sklearn [21] is a system designed to help machine learning users by automatically searching through the joint space of sklearn's learning algorithms and their respective hyperparameter settings to maximize performance using a state-of-the-art Bayesian optimization method. Auto-sklearn addresses the model selection problem by treating all of sklearn algorithms as a single, highly parametric machine learning framework, and using Bayesian optimization to find an optimal instance for a given dataset. Auto-sklearn also natively supports parallel runs (on a single machine) to find good configurations faster and save the n best configurations of

each run instead of just the single best. Nevertheless, and to the best of our knowledge Auto-sklearn does not provide support for neural networks and it does not take into consideration the complexity of the proposed models for assesing their optimality.

IV. An evolutionary algorithm for the neural network model selection problem

While there are a number of methods for automatic model selection and hyperparameter tuning, many of them do not provide support for some of the most sophisticated deep learning architectures. For instance, Auto-sklearn it does not provide good support for large machine learning problems, nor provides good support for distributed computing. Furthermore, Auto-sklearn lacks support for neural networks. Auto-keras and AutoML vision, which provide support for neural networks obtaining models with a high accuracy degree, do not consider the complexity (size) of the neural network when assessing the performance of the models. Furthermore, none of them provide support for regression problems.

We propose an efficient method that, given a dataset $\mathcal{D}$, will automatically find a neural network model that attains high performance while being computationally efficient. The proposed model is capable of performing inference tasks for both, classification and regression problems. Furthermore, the proposed system is scalable and easy to use in distributed computing environments, allowing it to be usable for large datasets and complex models, for such task we make use of Ray [22], a distributed framework designed with large scale distributed machine learning in mind.

Our method provides support for three of the major neural networks architectures, namely multilayer percpetrons (MLPs) [23], convolutional neural networks (CNNs) [24] and recurrent neural networks (RNNs) [25]. Our method can construct models of any of these architectures by stacking together a *valid* combination of any of the four following layers: fully connected layers, recurrent layers, convolutional layers and pooling layers. Our method does not only build neural networks for the aforementioned architectures, but also tunes some of its hyperparameters such as the number of neurons at each layer, the activation function to use or the dropout rates for each layer. Support for skip connections is left for future work.

We say that a neural network architecture is *valid* if it complies with the following set of rules, which we derived empirically from our practice in the field:

- A fully connected layer can only be followed by another fully connected layer
- A convolutional layer can be followed by a pooling layer, a recurrent layer, a fully connected layer or another convolutional layer
- A recurrent layer can be followed by another recurrent layer or a fully connected layer.
- The first layer is user defined according to the type of architecture chosen (MLP, CNN or RNN)
- The last layer is always a fully connected layer with either a softmax activation function for classification or a linear activation function for regression problems

A. The fitness function

To establish a ranking between the different tested architectures a suitable cost (fitness) function is required. While equation 2 can be used as the cost function, using it would give rise to a multi-objective optimization problem (MOP). We leave this approach for a future revision of this work and instead make use of scalarization to transform the MOP into a single- objective optimization problem (SOP). The scalarization approach taken here is the well known weighted sum method [26], thus equation 2 is restated as:

$$f^* = \underset{f \in \mathcal{F}}{\operatorname{argmin}} \quad (1-\alpha)p(f) + \alpha w(f). \tag{3}$$

The cost function associated with equation 3 is,

$$c(f) = (1-\alpha)p(f) + \alpha w(f), \tag{4}$$

where $\alpha \in [0, 1]$ is a scaling factor biasing the total cost towards the size of the network or its performance. Equation 3 measures the cost in terms of performance and size of a given neural network f.

Note that making an accurate assessment of the inference performance, $p(f)$, of a neural network involves training f for a large number of epochs. Since the training process usually involves thousands of computations training every candidate solution and then assessing its performance becomes unfeasible. Instead we relax the training process for each of the candidate models by using a *partial train* which, in short, is training the model for a very small number of epochs (only a few tenths of them). This approach has been successfully tested in [35] since eventhough the models are just partially trained, a clear trend in terms of whether a model is promising or not can be clearly observed.

Let $A \in \mathcal{A}$ be a certain neural network architecture trained on set $\mathcal{D}_t$, let also $\mathcal{P}_A(\mathcal{D}_v)$ represent the performance of the neural network A when tested using validation set $\mathcal{D}_v$ and the user-defined metric m, where m is usually any of the metrics listed in Table XIV . Using k-fold cross-validation the average performance of the algorithm can be written as

$$p = \frac{1}{k}\sum_{i=1}^{k} \mathcal{P}_A(\mathcal{D}_v^i) \tag{5}$$

For measuring the complexity of the architecture we consider the number of trainable weights w of the neural network which is a good indicator of how complex the architecture is.

Using p and w we propose the following fitness function

$$f = p + \alpha w, \tag{6}$$

where $\alpha \in [0, 1]$ is a scaling factor that indicates how much does the number of trainable weights w affects the overall fitness of the neural network. By setting $\alpha = 1$ the preference is given to very compact architectures, while $\alpha = 0$ will only care about architectures that find the best possible value for p regardless of their complexity.

Computing the fitness of individuals using the current definitions of p and w posses a big problem though, namely that the performance definition p and the number of weights

w are on entirely different scales. While w can range from a few hundreds up to several millions, the range of p is

$$p \in \begin{cases} [0, \inf], \text{if } m \text{ is } R^2 \\ [0, 1], \text{otherwise.} \end{cases} \tag{7}$$

As can be observed, even p can be in different ranges, it is necessary for our application that the range of p is consistent no matter the type of metric m, thus, in the case m is the R^2 metric we normalize the values of m to be within the range $[0, 1]$. The normalization process is quite straightforward: assuming a population $\mathcal{C}$ with n_s individuals, take the maximum value m_{max} for m at the population, then divide every individual in $\mathcal{C}$ by m_{max}. Following this process $p \in [0, 1]$ for any of the metrics m.

Now we focus on w. For the sake of simplicity lets just consider the case of the MLP class of neural networks since this is usually the model where w is larger. Let l_{max} be the maximum number of possible layers for any model, for this work we will limit $l_{max} = 64$ since we consider this a pretty decent number for most of the mainstream deep learning models. From Table XV we know that the maximum number of neurons at any layer is 1024, thus the maximum number of w, which we will call w_{max} for any given model is $w_{max} = 1024^2 \times 64 = 2^{26}$. Furthermore, we want neural networks that are similar (by a few thousands of weights) to have the same score w, therefore we discard the last 3 digits of the neural network and replace them by 0s, therefore let w^+ be this new weight with the last 3 digits discarded. Let $w^* = log(w^+)$, therefore $w^*_{max} \approx log(2) * 26$, hence we assume $w^* \in [0, 7.8]$.

Thus, we redefine Equation 6 as

$$f = 5p + \alpha w^*. \tag{8}$$

As can be observed, Equation 8 is now properly scaled, and therefore it is a suitable choice as the fitness function for assessing the performance of a neural network model.

B. Automatic Model Selection (AMS)

The key idea of our method is to develop an evolutionary algorithm (EA) capable of trying and evolving different neural network architectures and, in the end, find a suitable model for the given problem while being computationally efficient. EAs were chosen for this work since, contrary to the more classical optimization techniques, they do not make any assumptions about the problem, treating it as a black box that merely provides a measure of quality given a candidate solution, furthermore, they do not require the gradient when searching for optimal solutions making them very suitable for applications such as the one at hand.

In the following we describe the very basics of evolutionary algorithms as an introduction for the reader.

Every evolutionary algorithm consists of a population of individuals (sometimes EAs are also referred as population based algorithms) where each individual in the population (in this case neural network model) is indeed a potential solution to the optimization problem (in this case the CASH problem). Every individual has a specific encoding, in the evolutionary algorithm domain, that represents a solution to the given problem while the actual representation of the individual, in the specific application domain, is often referred as the phenotype. In particular, for this application the fenotype represents the neural network architecture while the genotype is represented by a list of lists. To assess the quality of an individual EAs make use of a so-called fitness function, which indicates how does every individual in the population performs with respect to a certain metric, establishing thus an absolute order among the various solutions and a way of fairly comparing them against each other.

New generation of solutions are generated iteratively by using crossover and mutation operators. Crossover operator is an evolutionary operator used to combine the information of two parents to generate new offspring while the mutation operator is used to maintain genetic diversity from one generation of the population to the next.

The basic template for an evolutionary algorithm is the following

Algorithm 1 Basic Evolutionary Algorithm

```
Let t = 0 be the generation counter
Create and initialize an n_x-dimensional population, C(0), to consist of n_s individuals
while stopping condition not true do
    Evaluate the fitness, f(x_i(t)), of each individual, x_i(t)
    Perform reproduction to create offspring
    Select the new population, C(t+1)
    Advance to the new generation, i.e. t = t + 1
end while
```

One of the major drawbacks of EAs is the time penalty involved in evaluating the fitness function. If the computation of the fitness function is computationally expensive, as in this case, then using any flavor of EA may be very computationally expensive and in some instances unfeasible. Micro-genetic algorithms [27] are one variant of GAs whose main difference is the use of small populations (less than 10 individuals per population) in contrast to some well established EAs like the genetic algorithms (GAs), evolutionary strategies (ES) and genetic programming (GP) [23]. Since computational efficiency is one of our main concerns for this work we will follow general principles of micro-GA in order to reduce the computational burden of the algorithm.

Specifically speaking and taking inspiration from the micro-GA the pseudocode for our proposed algorithm is described in Algorithm 2. Let C_p and M_p be the crossover and mutation probabilities respectively, let also G_{max} be the maximum number of allowed generations and E_{max} the maximum number of repetitions for the micro-GA, finally let $\mathcal{B}$ be an archive for storing the best architectures found at every run of the micro-GA. Our Algorithm is as follows

C. Encoding neural networks as genotypes

In order to perform the optimization of neural network architectures a suitable encoding for the neural networks is

Algorithm 2 Neural Network Evolution

Let $t_e = 0$ be the experiments counter
while $t_e < E_{max}$ **do**
  Let $t_g = 0$ be the generation counter
  Create and initialize an initial population $\mathcal{C}(0)$, consisting of n_s individuals, where $n_s <= 10$. See section IV-D
  while $t_g < G_{max}$ or nominal convergence not reached **do**
    Check for nominal convergence in $\mathcal{C}(t)$. See section IV-H
    Evaluate the fitness, $f(\mathbf{x}_i(t))$, of each individual, $\mathbf{x}_i(t)$. See section IV-A
    Identify best and worst individuals of $\mathcal{C}(t)$
    Replace worst individual in $\mathcal{C}(t)$ with best from $\mathcal{C}(t-1)$
    Perform selection. See section IV-E
    Perform crossover of individuals in $\mathcal{C}(t)$ with $C_p = 1$. Let $\mathcal{O}(t)$ be the offspring population. See section IV-F
    For each individual in $\mathcal{O}(t)$ perform mutation with M_p probability. See section IV-G
    Make $\mathcal{C}(t+1) = \mathcal{O}(t)$
    $t_g = t_g + 1$
  end while
  Append best solution from previous run to $\mathcal{B}$
  $t_e = t_e + 1$
end while
Final Solution is best existing solution in $\mathcal{B}$

needed. A good encoding has to be flexible enough to represent neural network architectures of variable length while also making it easy to verify the *validity* of a proposed neural network architecture.

Array based encodings are quite popular for numerical problems, nevertheless they often use a fixed-length genotype which is not suitable for representing neural network architectures. While it is possible to use an array based representation for encoding a neural network, this would require the use of very large arrays, furthermore verifying the validity of the encoded neural network is hard to achieve. Three-based representation as those used in genetic programming [23] enables more flexibility when it comes to the length of the genotype, nevertheless imposing constraints for building a valid neural network requires traversing the entire tree or making use of complex data structures every time a new layer is to be stacked in the model.

For this work, we introduce a new list-based encoding, that is, the genotype is represented as a list of arrays, where the length of the list can be arbitrary. Each array within the list represents the details of a given layer as described in Table XV. A visual depiction of the array is presented in Figure 1.

Layer type	Neuron number	Activation function	CNN filter size	CNN kernel size	CNN stride	Pooling size	Dropout rate

Fig. 1: Visual representation of a neural network layer as an array.

Let us illustrate the proposed encoding with an example, let S_e be a model composed of several stacked layers as those shown in Figure 1.

$$S_e = [[1, 264, 2, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0.65], [1, 464, 2, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0.35], [1, 872, 2, 0, 0, 0, 0, 0], [1, 10, 3, 0, 0, 0, 0, 0]]$$

The neural network representation of the model just presented is described in Table I.

Layer type	Neurons	Activation Function	Dropout Ratio
Fully connected	264	ReLU	n/a
Dropout	n/a	n/a	0.65
Fully Connected	464	ReLU	n/a
Dropout	n/a	n/a	0.35
Fully Connected	872	ReLU	n/a
Fully Connected	10	Softmax	n/a

TABLE I: Neural network model.

Encoding the neural network as a list of arrays presents two big advantages over other representations. First, the number of layers that can be stacked is, in principle, arbitrary. Second, the validity of an architecture can be verified in constant time every time a new layer is to be stacked to the model, this is due to the fact that in order to stack a layer in between the model one just needs to verify the previous layer and the layer ahead to check for compatibility. The rules for stacking layers together are described in Table XVI. As can be observed, the ability of stacking layers dynamically and verifying its correctness as a new layer is stacked allows for a powerful representation that can build several kinds of neural networks such as fully connected, convolutional and recursive.

D. Generating valid models

Generating valid models is straightforward. An initial layer type has to be specified by the user, the initial layer type can be FullyConnected, Convolutional or Recurrent. As it can be seen, defining the initial layer type effectively defines the type of architectures that can be generated by the algorithm, i.e. if the user chooses FullyConected as the initial layer, all the generated models will be fully connected, if the user chooses Convolutional as initial layer the algorithm will generate Convolutional models only and so on.

Just as the initial layer type has to be defined in advance, the final/output layer is also defined in advance, in fact, all of the generated models share the same output layer. The output layer is always a FullyConnected layer, furthermore, it is generated based on the type of problem to solve (classification or regression). In the case of classification problems the number of neurons is defined by the number of classes in the problem and the softmax function is used as activation function. For regression problems the number of neurons is one and the activation function used is the linear function.

Having defined the architecture type and the output layer generating an initial model is an iterative process of stacking new layers that comply with the rules in Table XVI. A user defined parameter m_l is used to stop inserting new layers,

every time a new layer is stacked in the model a random number $n_r \in [0, 1]$ is generated, if $n_r < m_l$ and if the current layer is compatible with the last layer (according to Table XVI) then no more layers are inserted. With regards to layers that have an activation function, even though in principle any valid combination is possible, for this application we choose to keep all the activations for similar layers the same across the model since this is usually the common practice.

E. Selection

In order to generate n_s offsprings $2n_s$ parents are required. The parents are chosen using a selection mechanism which takes the population $\mathcal{C}(t)$ at the current generation and returns a list of parents for crossover. For our application, the selection mechanism used is based on the binary tournament selection [23], [27]. A description of the mechanism is given next:

- Select n_p parents at random where $n_p < n_s$.
- Compare the selected elements in a pair-wise manner and return the most fit individuals.
- Repeat the procedure until $2n_s$ parents are selected.

It is important to note in the above procedure that the larger n_p is, the more the probable that the best individual in the population is chosen as one of the parents, this is not a desirable behavior, thus we warn the users to keep n_p small. Also, recall from Algorithm 2 that our approach uses elitism, therefore the best individual of a current generation goes unchanged in the next generation.

F. Crossover operator

Since the encoding chosen for this task is rather peculiar, the existing operators are not suitable for our encoding. In this section we describe in detail the used crossover operator. Our operator is based on the two point crossover operator for genetic algorithms [28] in the sense that two points are selected for each parent, nevertheless our operator is more restrictive in order to ensure the generation of valid architectures. The selection mechanism is described in Algorithm 3. The following algorithm will be executed for n_s times, where n_s is a user defined parameter, at most or until a valid offspring is generated. Nevertheless, based on our experience with the algorithm it usually takes only 1 attempt to successfully generate a valid offspring. Finally we would like to note that although this is the implementation we used, it may not be the only one to achieve the expected results.

In Algorithm 3 when we mean compatibility between two points we mean that such two points can be interchanged and still comply with the building rules stated in Table XVI. Let us illustrate Algorithm 3 with an example. Consider the following models

$$S_1 = [[1, 264, 2, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0, 0.65],\\ [1, 464, 2, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0, 0.35],\\ [1, 872, 2, 0, 0, 0, 0, 0], [1, 10, 3, 0, 0, 0, 0, 0]]$$

Algorithm 3 Crossover Method

Let S_1, S_2 be the arrays containing the stacked layers of a neural network model in parents 1 and 2 respectively.
Take two random points (r_1, r_2) from S_1 where $r_1 <= r_2$
if $r_1 = r_2$ **then**
  $r_2 = len(S_1 - 1)$
else
  pass
end if
Find all the compatible pairs of points $(r_3, r_4)_i$ in S_2 that are compatible with (r_1, r_2) where $r_3 < r_4$ and $r_4 - r_3 < l_{max}$
Randomly pick any of the pairs $(r_3, r_4)_i$
Replace the layers in S_1 between r_1, r_2 inclusive with the layers in S_2 between r_3, r_4 inclusive. Label the new model as S_3
Rectify the activation functions of S_3 to match the activation functions of S_1

$$S_2 = [[1, 56, 0, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0, 0.25],\\ [1, 360, 0, 0, 0, 0, 0, 0], [1, 480, 0, 0, 0, 0, 0, 0]\\ [1, 88, 0, 0, 0, 0, 0, 0], [5, 0, 0, 0, 0, 0, 0, 0, 0.2],\\ [1, 10, 3, 0, 0, 0, 0, 0]]$$

Lets take $r_1 = 1$ and $r_2 = 3$, since these points are going to be removed from the model then we need to find the compatible layers with $S_1[r_1 - 1]$ and $S_1[r_2]$ according to the rules described in Table XVI. Note however that if $r_1 = 0$, i.e. the initial layer, then only a layer whose layer type is equal to the layer type of $S_1[0]$ is compatible. Thus, for this example the compatible pairs of points $(r_3, r_4)_i$ are:

$$[(0, 0), (0, 2), (0, 4), (0, 5), (1, 2), (1, 4), (1, 5),\\ (2, 2), (2, 4), (2, 5), (4, 4), (4, 5), (5, 5)]$$

Now assume we pick at random the pair $(2, 4)$, thus the offspring which we will for simplicity call S_3 looks like:

$$S_3 = [[1, 264, 2, 0, 0, 0, 0, 0], [1, 360, 2, 0, 0, 0, 0, 0],\\ [1, 480, 2, 0, 0, 0, 0, 0], [1, 88, 2, 0, 0, 0, 0, 0],\\ [1, 872, 2, 0, 0, 0, 0, 0], [1, 10, 3, 0, 0, 0, 0, 0]]$$

which is indeed a valid model, the reader can check the actual model representations for each of the models in this example in Tables XVIII to XX. Notice though that all the activation functions of the same layer types are changed to match the activation functions of the first parent S_1, this is what we call activation function rectification, which basically means changing all the activation functions of the layers that share the same layer type between S_1 and S_3 to the activation functions used in S_1.

We would like to highlight one important feature of this crossover operator, namely that it has the ability to generate neural network models of different sizes, i.e. it can shrink or increase the size of one of the parents. This is a desirable

behavior as in real life, machine learning experts will often try various sizes of neural network models when trying to find the one that has the best inference capabilities.

G. Mutation operator

The mutation operator is used to induce small changes to some of the models generated through the crossover mechanism. In the realm of evolutionary computation these subtle changes tend to improve the exploration properties of the current population (genetic diversity) by injecting random noise to the current solutions. Although according to [27] mutation is not needed in the micro-GA, we believe some sort of mutation is needed in our application in order to get more diverse models which could potentially lead to better inference abilities, nevertheless, our mutation approach will be less disruptive in order to mitigate its effect. Following the same ideas found on the literature we developed a mutation operator to handle neural network models.

As stated above our mutation approach is less disruptive than the common mutation operators [23], this decision follows two main reasons: First, is the fact that usually micro genetic algorithms don't make use of the mutation algorithm since the crossover operator has already induce significant genetic diversity in the population. The second reason is related to the way neural networks are usually built by human experts, commonly experts try a number of models and then make subtle changes to each of them in order to try to improve the inference ability of them, such changes usually involve changing the parameters in a layer, adding or removing a layer, adding regularization or changing the activation functions.

Based on the principles described above, our mutation process randomly chooses one layer, using a probability m_p, of the model and then proceeds to make one of the following operations:

- Change a parameter of the layer chosen for a value complying the values stated in Table XV.
- Change the activation function of the layer. This would involve rectifying the entire model (described in section IV-F).
- Add a dropout layer if the chosen layer is compatible.

This operations together provide a rich set of possibilities for performing efficient mutation while still keeping valid models after mutation is performed.

H. Determining nominal convergence

Nominal convergence is one of the criteria used for early stopping of the evolutionary procedure of our algorithm. Some literature defines the convergence in terms of the fitness of the individuals [23], while in [27] the convergence is defined in terms of the genotype or phenotype of the individuals. Although convergence based on the actual fitness of the individuals may be easier to asses given that the fitness is already calculated, we believe that an assessment of convergence based on the actual genotype of the individuals suits our needs better, this follows the following reasoning.

Since neural networks are stochastic in nature, we expect some variations in the fitness of the individuals at every different run, furthermore since we are running the training process for only few epochs (in order to avoid a high computational burden) the performance of the networks can be quite different and would not be a reliable indicator of convergence. Instead, to assess convergence we look at the genotype and compute the similarities between the different individuals.

To compute the similarities between different individuals we take the following approach. Let S_1, S_2 where $len(S_2) >= len(S_1)$ be the genotype representing two different models, let also $S_1 - S_2$ represent the layer-wise difference between each model and $S_i[j]$ be the array representation of the $j - th$ layer of model i, $S_2 - S_1$ is defined in Algorithm 4.

Algorithm 4 $S_2 - S_1$ Method

Let $d \in \mathbb{R}$ be the distance between the two models. Make $d = 0$
for Each layer i in S_1 except last layer **do**
  $d = d + norm_2(S_2[i] - S_1[i])$
end for
for Each remaining layer i in S_2 except last layer **do**
  $d = d + norm_2(S_2[i])$
end for
Return d

This method is computationally inexpensive since the size of the population is small. Furthermore, it helps accurately establish the similarity between any two neural networks, given two neural network models S_1 and S_2 is $S_1 = S_2$ then $S_2 - S_1 = 0$. For our purposes we stop the algorithm and launch the new experiment if the distance between any s models is smaller than c where both s and c are user defined parameters.

I. Implementation

AutoNN is implemented in about 700 lines of code in Python. The code can be found in https://github.com/dlaredo/automatic_model_selection. We took a functional programming approach for its implementation. The models S_i generated by the algorithm are fetched to Keras [5] and then evaluated, nevertheless the models can be evaluated in any other framework such as TensorFlow or Pytorch and even using different programming languages such as C++ for performance reasons.

In order to boost performance we make use of Ray [22] which is a distributed computing framework tailored for AI applications. In order to distribute workloads in Ray developers only have to define Remote Functions make use of Python annotations, Ray will then distribute these Remote Functions across the different nodes in the cluster. There are three different types of nodes in Ray: Drivers, Workers and Actors. A Driver is the process executing the user program, a Worker is a stateless process that executes remote functions invoked by a driver or another worker, finally, an Actor is a

statefull process that executes, when invoked, the methods it exposes.

For our implementation we code the individual fetching to Keras and its fitness evaluation as Ray Remote Functions (Workers), while the rest of our algorithm is implemented within the Driver, therefore the partial train of each neural network within the current population is performed in a distributed way, highly increasing the performance of our algorithm. Furthermore since the only messages being sent over the cluster are arrays (the neural network representation S_i) and the fitness of the neural network model f there is little chance that the data interchanged causes a bottleneck or increases latency in the system.

V. Evaluation

We evaluate AutoNN with two different datasets, each of which is a different type of inference problem. Our results are compared against baseline implementations and state-of-the-art methods for automatic model selection. In particular we compare our results against AutoWeka [18], PyBrain [2] and MLLib [3].

For the experiments in this section each model generated by AMS was trained using the following parameters:

Dataset	Epochs	Learning Rate	Optimizer	Loss function	Metrics
MNIST	5	0.001	Adam	Categorical crossenthropy	Categorical accuracy
CMAPSS	5	0.01	Adam	MSE	MSE
CIFAR10	5	0.001	Adam	Categorical crossenthropy	Categorical accuracy

TABLE II: Training parameters for each of the used datasets.

For CMAPSS dataset we used a larger learning rate since we are evaluating the model using very few epochs for this complex problem, therefore, in order to get a clearer idea of which individuals within the population may be promising we speed up the training process by increasing the learning rate.

A. MNIST Dataset - A classification problem

We first test our algorithm on the MNIST Dataset [29]. The MNIST Dataset of handwritten digits is one of the most commonly used datasets for evaluating the performance of neural networks. It has a training set of 60,000 examples and a test set of 10,000 examples. The digits have been size-normalized and centered in a fixed-size image, the size of each image is of 28x28 pixels. Ass part of the data pre-processing step we normalized all the pixels in each image to be in the range of $[0, 1]$ and unrolled the 28x28 image into a vector with 784 components.

We use MNIST dataset as a baseline for measuring the performance of our approach, furthermore, we use MNIST to analyze each one of the major components of AutoNN. Given the popularity of MNIST, several neural networks with varying degrees of accuracy have been proposed, therefore it is easy to find good models to compare with.

We start by running AutoNN to find a suitable FullyConnected model for classification for the MNIST dataset. The details for the parameters used in this test are described in Table III

Parameter	AutoNN Value
Problem Type	1
Architecture Type	FullyConnected
Input Shape	$(784, M)$
Output Shape	$(10, M)$
Cross Validation Ratio	$c_v = 0.2$
Mutation Ratio	$m_p = 0.4$
More Layers Probability	$n_r = 0.7$
Network Size Scaling Factor	$\alpha = 0.8$
Population Size	$n_s = 10$
Tournament Size	$n_t = 4$
Max Similar Models	$s = 3$
Total Experiments	$E_{max} = 5$

TABLE III: Parameters for MNIST for each method.

We first take a look at the generated initial population. For the sake of space we will only discuss the sizes of the models, furthermore we will make a small change in our notation for describing neural network models, for the remainder of this section we denote a layer of a neural network as (n_e, a_f) where n_e denotes the number of neurons in case the layer is fully connected or the dropout rate in case the layer is a dropout layer and a_f denotes the activation function of the later if the layer is a fully connected layer. The initial five generated individuals are presented next. Fitness, accuracy and raw size of the models in the initial population are presented in Table IV

$$
\begin{aligned}
S_1 &= [(280,1),(32,1),(0.4),(304,1),(96,1),\\
&\quad (0.55),(600,1),(10,3)]\\
S_2 &= [(96,0),(0.55),(168,0),(10,3)]\\
S_3 &= [(1024,2),(560,2),(0.15),(360,2),(624,2),\\
&\quad (0.5),(144,2),(616,2),(504,2),(776,2),(0.3),\\
&\quad (8,2),(200,2),(0.2),(904,2),(0.35),(664,2),\\
&\quad (0.35),(904,2),(0.65),(488,2),(0.4),(448,2),\\
&\quad (216,2),(336,2),(368,2),(400,2),(0.2),\\
&\quad (112,2),(48,2),(0.3),(944,2),(584,2),(128,2),\\
&\quad (0.15),(376,2),(288,2),(816,2),(10,3)]\\
S_4 &= [(672,0),(840,0),(0.25),(384,0),(400,0),\\
&\quad (712,0),(10,3)]\\
S_5 &= [(472,1),(968,1),(0.4),(816,1),(104,1),\\
&\quad (0.5),(488,1),(192,1),(0.4),(256,1),(10,3)]
\end{aligned}
$$

Model	Score (Accuracy)	Trainable Parameters	Fitness
S_1	94.6%	332314	4.9519
S_2	91.5%	93346	4.1827
S_3	10.5%	6305682	14.3839
S_4	92.0%	1862426	5.8084
S_5	95.0%	1901162	5.5140

TABLE IV: Scores for the initial population found by AutoNN for MNIST. $\alpha = 0.8$

First thing we can observe is that the sizes of the models are widely variable, with some models having as few as 1 hidden layer and some having more than 20 hidden layers, another

thing to note is the variability in terms of activation functions with some models using sigmoid, some using tanh and some using relu as activation functions.

The next thing to notice is the fitness of each of the initial individuals with the worst individual in the population (S_3) being extremely unfit due to the large size of the network (more than 6 million trainable parameters) and the low accuracy of the model (about 10%). The rest of the individuals display a decent accuracy (about 90% of accuracy) but they exhibit a large number of trainable parameters. Since MNIST is a simple dataset to infer for modern neural networks it is observable that most of the neural networks at the initial population already attain acceptable accuracy, nevertheless in this specific case, the size of the network can be greatly improved. In the next sections we will show how AMS optimizes the accuracy along with the size of the models for more complex datasets.

For this test, after the 10 generations, the algorithm converged to $S_1^* = [(96, 1), (10, 3)]$, where * denotes the best individual in the population and the subindex denotes the experiment number.

We now run the same experiment four more times for a total of five different experiments with the same parameter settings for AMS. The obtained models are presented next, the fitness, accuracy and raw size of the models are presented in Table V. The best overall model is $S^* = S_2^*$.

$$
\begin{aligned}
S_1^* &= [(96, 1), (10, 3)] \\
S_2^* &= [(48, 2), (48, 2), (10, 3)] \\
S_3^* &= [(408, 2), (10, 3)] \\
S_4^* &= [(296, 1), (10, 3)] \\
S_5^* &= [(128, 1), (128, 1), (0.3), (10, 3)]
\end{aligned}
$$

Model	Score (Accuracy)	Trainable Parameters	Fitness
S_1^*	94.4%	76330	4.4638
S_2^*	95.0%	40522	4.1827
S_3^*	96.8%	224370	4.7226
S_4^*	95.1%	235330	4.7843
S_5^*	95.5%	118282	4.5016

TABLE V: Scores for the best models found by AutoNN for MNIST. $\alpha = 0.8$

As can be observed in Table V small models are preferred, furthermore there seems to be a preference for tanh activation functions. The fact that small models are preferred over larger models, despite the fact that larger models may yield better performance, is due to the value of the weighting factor $\alpha = 0.8$ which highly penalizes the overall size (number of trainable parameters) of the neural network. Let us further illustrate this behavior by running the algorithm with $\alpha = 1$ and $\alpha = 0.6$.

The best models for each experiment with $\alpha = 0.6$, are listed next, the fitness and raw size of the models are described in Table VI. The best overall model is $S^* = S_5^*$.

$$
\begin{aligned}
S_1^* &= [(312, 2), (10, 3)] \\
S_2^* &= [(368, 2), (0.15), (10, 3)] \\
S_3^* &= [(200, 1), (10, 3)] \\
S_4^* &= [(224, 2), (10, 3)] \\
S_5^* &= [(88, 2), (88, 2), (10, 3)]
\end{aligned}
$$

Model	Score (Accuracy)	Trainable Parameters	Fitness
S_1^*	96.7%	248050	3.5575
S_2^*	96.8%	292570	3.5976
S_3^*	96.3%	159010	3.4891
S_4^*	96.3%	178090	3.5169
S_5^*	95.2%	77802	3.4094

TABLE VI: Scores for the best models found by AutoNN for MNIST, $\alpha = 0.6$.

The results in Table VI display larger models with respect to those displayed in Table V. This is due to the relaxation on the α parameter which takes more into account the accuracy of the model rather than the size of the network itself. Nevertheless, it can be observed that the accuracy of the obtained models when $\alpha = 0.6$ is just slightly better than the results obtained with $\alpha = 0.8$, this is likely due to the fact that MNIST dataset is usually easy to classify using neural networks. We will further analyze this behavior using other datasets in the next sections.

Next we repeat the experiment with $\alpha = 1$, again the obtained models are listed next and their fitness and raw size of the models are described in Table VII. The best overall model is $S^* = S_2^*$.

$$
\begin{aligned}
S_1^* &= [(136, 2), (136, 2), (0.35), (10, 3)] \\
S_2^* &= [(32, 1), (32, 1), (10, 3)] \\
S_3^* &= [(56, 2), (0.1), (10, 3)] \\
S_4^* &= [(152, 1), (152, 1), (10, 3)] \\
S_5^* &= [(64, 2), (10, 3)]
\end{aligned}
$$

Model	Score (Accuracy)	Trainable Parameters	Fitness
S_1^*	96.5%	126762	5.4529
S_2^*	93.9%	26506	5.0388
S_3^*	94.1%	44530	5.2348
S_4^*	96.0%	144106	5.5550
S_5^*	94.6%	50890	5.2475

TABLE VII: Scores for the best models found by AutoNN for MNIST, $\alpha = 1$.

The results in Table VII show that when the number of trainable parameters has a large impact on the overall fitness of the individuals, the algorithm tends to prefer smaller networks, this is specially useful for cases where the computational power is limited, such as embedded systems. This brings an obvious drawback, namely that neural networks that exhibit a lower performance as compared to larger neural networks may

be preferred. Nevertheless, this tradeoff can be controlled by the user by varying the α parameter.

Note that the change in fitness among the three experiments is due to the fact that the size of the neural network was scaled (See equation 8) and thus there is no fair way of comparing the fitness of the models shown Tables V, VI and VII against each other.

Finally, we compare the best models for each value of α against each other. A 10-fold cross-validation process, with a training of 50 epochs per fold, was carried out for each one of the best models in order to obtain the mean accuracy for each model. We denote S_1^* as the best model corresponding to $\alpha = 0.6$, S_2^* is the model corresponding to $\alpha = 0.8$ and S_3^* is the model corresponding to $\alpha = 1$. We also measure the accuracy of each of the models using a test set that was never used during the training or tuning processes of the models. The accuracy averages and size of the networks are summarized in Table VIII. The experiments for each α value took about 8.5 minutes in our test rig.

Model	10-fold Avg. Score	Test Avg. Score	Network size
S_1^*	97.6%	97.7%	93346
S_2^*	97.0%	97.2%	77802
S_3^*	96.1%	96.4%	26506

TABLE VIII: Accuracy obtained by each of the top 3 models for MNIST dataset.

As expected, model S_3^* yields a smaller neural network (about 3 times smaller) than the rest of the proposed models, nevertheless its accuracy is the worst of the three models (though by a small margin). On the contrary model S_1^* gets the best performance (again marginal) in terms of accuracy but with a larger neural network as compared to model S_3^*. Finally, model S_2^* as expected, attains a performance in between S_1^* and S_3^* with a number of trainable parameters also in between S_1^* and S_3^*. It is important to note though that the accuracy of each of the models presented for this dataset is acceptable as compared against some modern methods. Table IX shows the top models along with their obtained accuracy for the MNIST dataset, it can be observed that the accuracy obtained by AMS is close to that obtained by fine tuned models. A thorough comparison between the obtained models and some other modern models using this dataset is out of the scope of this work mainly fue to the fact that the models obtained by AMS are not fine tuned as the models with higher accuracy.

Method	Test accuracy	Size
3 Layer NN, 300+100 hidden units [30]	96.95%	266610
2 Layer NN, 800 hidden units [31]	98.4%	636010
6-layer NN (elastic distortions) [32]	99.65%	11972510

TABLE IX: Top results for MNIST dataset.

Comparing the models obtained by AMS agains the models in Table IX we can observe that eventhough AMS models don't attain the highest accuracy they exhibit good inference capabilities with a much lesser number of trainable parameters (size of the model). This shows that AMS models show a good balance between the inference power of the model and its overall size, furthermore the score-size tradeoff can be controlled by means of the α parameter, where a value closer to $\alpha = 0$ makes AMS prefer networks with higher scores and a value closer to $\alpha = 1$ makes AMS prefer networks with smaller sizes.

B. CMAPSS Dataset - A regression problem

In this section we analyze the performance of AMS when working with regression problems. For testing regression we use the C-MAPSS dataset [33]. The C-MAPSS dataset contains simulated data produced using a model based simulation program developed by NASA. The dataset is further divided into 4 subsets composed of multi-variate temporal data obtained from 21 sensors, nevertheless for our test we will only make use of the first subset of data. Training and separate test sets are provided. The training set includes run-to-failure sensor records of multiple aero-engines collected under different operational conditions and fault modes.

The data is arranged in an $n \times 26$ matrix where n is the number of data points in each subset. The first two variables represent the engine and cycle numbers, respectively. The following three variables are operational settings which correspond to the conditions in Table X and have a substantial effect on the engine performance. The remaining variables represent the 21 sensor readings that contain the information about the engine degradation over time.

Train trajectories	Test trajectories	Operating conditions	Fault modes
100	100	1	1

TABLE X: CMAPSS dataset details.

Each trajectory within the training and test sets represents the life cycles of the engine. Each engine is simulated with different initial health conditions, i.e. no initial faults. For each trajectory of an engine the last data entry corresponds to the cycle at which the engine is found faulty. On the other hand, the trajectories of the test sets terminate at some point prior to failure, hence the need to predict the remaining useful life (RUL). The aim of the MLP model is to predict the RUL of each engine in the test set via regression. The actual RUL values of test trajectories are also included in the dataset for verification. Further discussions of the dataset and details on how the data is generated can be found in [34].

For this test we follow the data pre-processing described in [35], in short only 14 out of the total 21 sensors are used as the input data. Furthermore we also use a strided time-window, with window size of 24, a stride of 1 and earlyRUL of 129, to form the feature vectors for the MLP as in [35]. Further details of the time-window approach can be found in [35] and [36].

We run AMS to find a suitable FullyConnected model for regression using the CMAPSS dataset. The details for the parameter used in this test are described in Table XI

Once again we start by presenting the baseline for our tests. Table XII presents some of the top results obtained by MLPs in the CMAPSS dataset, the results are measured in terms of the RMSE (Root Mean Squared Error) between the real RUL and the predicted RUL.

Parameter	AutoNN Value
Problem Type	1
Architecture Type	FullyConnected
Input Shape	$(336, M)$
Output Shape	$(1, M)$
Cross Validation Ratio	$c_v = 0.2$
Mutation Ratio	$m_p = 0.4$
More Layers Probability	$n_r = 0.7$
Network Size Scaling Factor	$\alpha = 0.8$
Population Size	$n_s = 10$
Tournament Size	$n_t = 4$
Max Similar Models	$s = 3$
Total Experiments	$E_{max} = 5$

TABLE XI: Parameters for CMAPSS for each method.

Method	Test RMSE	Network size
Time Window MLP [37]	15.16	6041
Time Window MLP with EA [35]	14.39	7161
Deep MLP ensemble [38]	15.04	n/a

TABLE XII: Top results for CMAPSS dataset.

As with MNIST dataset we performed experiments for $\alpha \in \{0.6, 0.8, 1\}$. The best global models (best out of the five experiments) obtained for each of the α values are shown in Table XIII along with their scores for CMAPSS data (RMSE) and the sizes of the networks. S_1^* denotes the best model for $\alpha = 0.6$, while S_2^* and S_3^* denote the best models for $\alpha = 0.8$ and $\alpha = 1$ respectively. The experiments for each α value took about 3.5 minutes in our test rig.

Model	10-fold Avg. Score	Test Avg. Score	Network size
S_1^*	15.16	16.12	57809
S_2^*	15.20	14.83	9177
S_3^*	15.00	14.96	6817

TABLE XIII: RMSE obtained by each of the top 3 models for CMAPSS dataset.

The results presented in Table XIII further demonstrate the impact of the α parameter. As can be observed the size of the networks grow as α is relaxed (smaller). It can also be observed that the results obtained by the three proposed models in the Cross-Validation sets are very close among each other, nevertheless it is important to point out that S_1^* attained such score with a larger network as compared with S_2^* and S_3^* whose sizes are fairly similar. This is mainly because the CMAPSS dataset does not require very large neural networks, therefore small models are usually preferred.

The obtained models are also competitive when compared against some of the latest MLPs used with CMAPSS dataset (XII). In this case we compare against the score obtained in the test set for each of the models. It is shown that two of the three models obtained by AMS obtain a better score than two (Time Window MLP and Deep MLP ensemble) of the three compared models, furthermore, the sizes of the proposed networks are as small as the sizes of the compared models.

VI. Conclusions and Future Work

In this paper we presented AutoNN, a new evolutionary algorithm for efficiently finding suitable neural network models for both classification and regression problems. Making use of efficient mutation and crossover operators the AutoNN is able to generate valid and efficient neural networks, in terms of both the size of the network and its performance. Furthermore, AutoNN is intrinsically distributable, exploiting this feature with the use of Ray [22] we were able to find efficient models for the MNIST dataset [29].

Future work will consider more complex neural network architecturs such as LSTM and CNNs, techniques for assembling entire neural network pipelines will also be explored in future as well as the inclusion of more hyperparameters in the tuning process. Finally a better way of measuring distance between two neural network architectures will be explored, since this last element is of high importance for applications such as visualization and evolutionary computation.

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Metric name	Definition
Root Mean Squared Error	Regression
Accuracy	Classification
Precision	Classification
Recall	Classification
F1	Classification

TABLE XIV: Common performance metrics for neural networks

Cell number	Cell name	Data Type	Represents	Applicable to	Values
0	Layer type	Integer	The type of layer. See table XVI	MLP/RNN/CNN	$x \in \{1, \ldots, 5\}$
1	Neuron number	Integer	Number of neurons/units in the layer	MLP/RNN	$8 * x$ where $x \in \{1, \ldots, 128\}$
2	Activation function	Integer	Type of activation function. See table XVII	MLP/RNN/CNN	$x \in \{1, \ldots, 4\}$
3	Filter size	Integer	Number of filters generated by the layer	CNN	$8 * x$ where $x \in \{1, \ldots 64\}$
4	Kernel size	Integer	Size of the kernel used for convolutions	CNN	3^x where $x \in \{1, \ldots, 6\}$
5	Stride	Integer	Stride used for convolutions	CNN	$x \in \{1, \ldots, 6\}$
6	Pooling size	Integer	Size for the pooling operator	CNN	2^x where $x \in \{1, \ldots 6\}$
7	Dropout rate	Float	The dropout rate applied to the following layer	MLP/RNN/CNN	$x \in [0, 1]$

TABLE XV: Details of the representation of a neural network layer as an array.

Layer type	Layer name	Can be followed by
1	Fully connected	$[1, 5]$
2	Convolutional	$[1, 2, 3, 5]$
3	Pooling	$[1, 2]$
4	Recurrent	$[1, 4]$
5	Dropout	$[1, 2, 4]$

TABLE XVI: Neural network stacking/building rules.

Index	Activation function
0	Sigmoid
1	Hyperbolic tangent
2	ReLU

TABLE XVII: Available activation functions.

Layer type	Neurons	Activation Function	Dropout Ratio
Fully connected	264	ReLU	n/a
Dropout	n/a	n/a	0.65
Fully Connected	464	ReLU	n/a
Dropout	n/a	n/a	0.35
Fully Connected	872	ReLU	n/a
Fully Connected	10	Softmax	n/a

TABLE XVIII: Neural network model corresponding to S_1.

Layer type	Neurons	Activation Function	Dropout Ratio
Fully connected	56	Sigmoid	n/a
Dropout	n/a	n/a	0.25
Fully Connected	360	Sigmoid	n/a
Fully Connected	480	Sigmoid	n/a
Fully Connected	80	Sigmoid	n/a
Dropout	n/a	n/a	0.20
Fully Connected	10	Softmax	n/a

TABLE XIX: Neural network model corresponding to S_2.

Layer type	Neurons	Activation Function	Dropout Ratio
Fully connected	264	ReLU	n/a
Fully Connected	360	ReLU	n/a
Fully Connected	480	ReLU	n/a
Fully Connected	88	ReLU	n/a
Fully Connected	872	ReLU	n/a
Fully Connected	10	Softmax	n/a

TABLE XX: Neural network model corresponding to S_3.