GROWING AN ARCHITECTURE FOR A NEURAL NETWORK

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Abstract. We propose a new kind of automatic architecture search algorithm. The algorithm alternates pruning connections and adding neurons, and it is not restricted to layered architectures only. Here architecture is an arbitrary oriented graph with some weights (along with some biases and an activation function), so there may be no layered structure in such a network. The algorithm minimizes the complexity of staying within a given error. We demonstrate our algorithm on the brightness prediction problem of the next point through the previous points on an image. Our second test problem is the approximation of the bivariate function defining the brightness of a black and white image. Our optimized networks significantly outperform the standard solution for neural network architectures in both cases.

1. Introduction

(Artificial) deep neural networks are nowadays very popular algorithms aiming to imitate processes inside a human brain. They train by examples and are shown to be very effective for pattern recognition problems of different kinds. Despite an avalanche of applications, much is unknown about neural networks from the mathematical point of view. Much is done by guessing and by whatever worked well in similar problems.

One important open problem is determining the best architecture for a neural network. For a layered network this means to determine the number of neurons and the number of layers for a neural network. Among the main approaches to automatic architecture search are the following. See also survey [13].

1. Empirical/statistical methods that choose the weights according to the effect they make on the model’s performance, see, e.g. [4].

2. Evolutionary algorithms that start with selecting parent networks, then proceed with combination and mutations, and selecting the best ones. The algorithms then repeat by assigning the best ones as new parents. See e.g. [3, 7, 15].

3. Pruning methods that start with a larger than necessary multilayer network and then remove neurons that have little contribution to the solution. There are several different ways to decide which neuron is not needed, see e.g. [18, 16, 6, 11, 5]. Pruning does not lead [20] to the increase of fault tolerance of the system. Among known disadvantages is that one usually does not know a priori how large the original network should be. Also starting with a large network could be excessively costly to trim the unnecessary units.

4. Constructive methods that start with an initial network of a small size, and then incrementally add new hidden neurons and/or hidden layers until some prescribed error requirement is reached or if no performance improvement can be observed, see e.g. surveys [10] (add a neuron, add a layer) [12], and e.g. papers [14, 1] 22.
Among known disadvantages of these methods is that the size of the obtained multilayer networks are reasonable but rarely “optimal”.

Cell-based methods create the architecture from a smaller-sized blocks, see e.g. [2, 21, 23].

Our growing architecture algorithm is a combination of ideas of both pruning and constructing algorithms. We also extend our domain to a more general one (that include layered networks as a particular case). For us an architecture is an arbitrary oriented graph with some weights (along with some biases and an activation function), so there may be no layered structure in such a network. We compare our optimized network with the large number of networks with standard architectures. We show that for the same error we can have a significantly smaller complexity.

In recent years, we have seen the ever-increasing efficiency of neural networks. At the same time, their complexity is growing. Here we measure the complexity of a neural network by the number of weights, the values of which are selected in the learning process. Those who do not work directly with neural networks usually expect the complexity of the network to be tens, hundreds, at most thousands. In reality, the complexity of modern neural networks is much higher. Thus, for the standard MNIST handwritten digit classification problem, the number of learnable parameters in the best networks is hundreds of thousands and millions, while there are only 60,000 training examples (small square 28 × 28 pixel grayscale images of handwritten single digits between 0 and 9).

Minimization of the network complexity is the goal of our work.

Most of our computations are realized in C++ instead of some conventional package (e.g. TensorFlow/Python). This is because layered architectures are the main objective of such specialized packages, and dealing with non-layered ones presents such difficulties that outweigh their conveniences.

The structure of the paper is as follows. In section 2 we introduce our notation. In section 3, we describe our “architecture growing” algorithm. In section 4, we present the results of our experiments with the brightness prediction problem and compare our algorithm with polynomial regression and standard neural networks. In section 6, we summarize our results.

2. Preliminaries. Architecture and complexity

Let \( f(\mathbf{x}, \mathbf{w}) \) be a function that represents a feedforward neural network, where \( \mathbf{x} \) be an input vector and \( \mathbf{w} \) be a vector of learnable parameters (weights). For regression tasks we minimize target function

\[
S = \sum (f(\mathbf{x}_i, \mathbf{w}) - y_i)^2.
\]  

We do not consider convolutional neural networks: all training vectors \( \mathbf{x}_i \) have a fixed length. The training dataset is represented in the form of a matrix \( A \), each line of which first contains the value \( y_i \), and then coordinates of the vector \( \mathbf{x}_i \).

Fully connected are layered networks where each neuron receives the values of all neurons from the previous layer. Our algorithm allows networks of even more general type, where every neuron receives all input values and also values from all previous neurons. We shall call such maximally fully connected. By changing weights, one can include layered fully and not fully connected networks into the network of such a general type. Each
neuron is a function of $\mathbb{R}^n \to \mathbb{R}$ of the form

$$(z_1, \ldots, z_n) \mapsto g(w_0 + w_1 z_1 + \ldots + w_n z_n)$$

where $(z_1, \ldots, z_n)$ are neuron’s input arguments, $(w_0, w_1, \ldots, w_n)$ are the corresponding weights and $g : \mathbb{R} \to \mathbb{R}$ is some activation function. In this paper we consider some most common ones, see details in section 4.3.

Hardware specification: Intel(R) Pentium(R) CPU G4500 @ 3.50GHz, 32G byte mem. and Intel(R) Core(TM) i7-8565U CPU @ 1.80GHz 16 G byte mem.

Software specification: Visual Studio 2019 Community (C++), Python 3.9.5, PyCharm 2019 Community Edition, Numpy 1.19.5, TensorFlow 2.5.0.

3. Architecture growing algorithm

The rough idea is to remove redundant connections in the neural network, while possible, and then to add a new neuron to its beginning, with running training processes in between. Then again remove some connections, while possible, and when it not possible, add a neuron, and so on. We first describe elements of the algorithm and then put it all together at the end of the section.

3.1. Connection removal procedure.

(1) Find three connections with the least (w.r.t. their absolute value) weights.

(2) Create three different networks, by removing one of these three connections in each case. In every case start the learning process for the resulting network to minimize $\ell$ within the specified time $\Delta$.

(3) Choose from the three reduced optimized networks the one with the smallest error and optimize it with training time $3\Delta$.

(4) While removing a connection, it may turn out that this connection is the only input connection for some neuron, i.e. it works by the formula

$$F(x_1) = f(w_0 + w_1 x_1) .$$

In this case, we remove such a neuron, and approximate its action by linear function

$$G(x_1) = v_0 + v_1 x_1 ,$$

where we choose $(v_0, v_1)$ s.t. to minimize the deviation

$$||G - F||^2 = \int_{t_0}^{t_1} (F(t) - G(t))^2 dt ,$$

where $[t_0, t_1]$ is the interval of values taken by the parameter $x_1$ for the whole training matrix.

(5) While removing a connection, it may turn out that the value of some neuron does not participate anymore in further calculations. We remove such a neuron.

Repeat the “one connection removal procedure” until the error increases by no more than $(1 + \varepsilon)$ times, where $\varepsilon$ is small enough. In our experiments $\varepsilon = 0.006$.

Remark 3.1. One might expect that by removing connections in a neural network, we increase its error. However, as we discovered, it is frequently not the case if the original network was not trained well enough. In such cases the quality of the “reduced” network
can be much improved after the optimization. Our experiments showed that in the beginning, when the connections are started to be removed, the error in the network almost does not grow until we reach a “saturation” point where any attempt to remove any further connection results in a noticeable increase of the error. The boundary 1.006 was chosen based on the results of these experiments.

3.2. **Adding a neuron procedure.** In the course of the algorithm, we run the connection removal procedure until the error increase is too large. After that we do the following.

1. Add one extra neuron to the very beginning of the neural network and connect it with all input parameters and with all other neurons of the original network.
2. Set all the weights of all new connections equal to 0. Thus, the computations in this new neural network go exactly by the same algorithm as in the original one, and the error will remain the same.
3. Retrain the new network with training time $5\Delta$. The error of the network decreases.

3.3. **Architecture growing algorithm.** We start with an arbitrary architecture and then execute the following procedure.

1. Remove all redundant connections as described in section 3.1.
2. If the complexity of the network reaches the preset limit, end the procedure.
3. Add a neuron as described in section 3.2.
4. Return to step (1).

On fig. 1 and fig. 2 are two typical graphs of the dependence of the error on the complexity that we obtain executing our algorithm. On fig. 1, the starting point of the algorithm is represented by the blue point above the start of $\leftarrow$. Removing connections, we move in the direction indicated by $\leftarrow$, from the right to the left: complexity decreases while the error slightly increases. At some moment, removing a connection leads to a sudden jump in error (see along vertical-ish arrow).

Once this happens we stop removing connections and add one more neuron. This moves us to the start of $\leftarrow$. From there we continue the process of removing connections (and thus move in the direction indicated by $\leftarrow$) until we reach the jump in error, and then the process repeats.

4. **Comparison with other approaches on brightness prediction problem**

To illustrate our idea, consider the brightness prediction problem for an image point knowing the brightness of several previous points.

4.1. **Neuro network built using our approach.** The data is kept in a table, where rows and columns are $x$ and $y$ coordinates of the point and values are the numbers from 0 to 255.

The previous points are ordered as shown in table 1. Here $Y$ is the current point, and the first column and the first row give the $(x, y)$-coordinates of the points relative to $Y$. The other numbers in the table indicate the order in which the points will be considered.
To normalize the numbers, we subtract from all values of $Y$ the brightness of the previous (left) point and divide all values by 100. So building the forecast by 5 points, there will be only 4 input parameters in the neural network. For the experiments we choose a graphics file of size $512 \times 512$. For 4 previous points, the resulting training file looks as in table 2. We present and compare the results of our experiments in table 4 and table 5.
4.2. For comparison: linear and polynomial approximation. As a starting point, we compare the performance of our optimized networks with the results obtained using linear/polynomial regressions:

\[ y_i \approx P_d(w, x_i) , \]
where $P_d$ is a polynomial in $\mathbf{x}_i$ of degree $d$, and $\mathbf{w}$ is the vector of weights. Table 3 contains the mean square errors (over all points of the image) in such approximation with polynomials of degrees 1, 2, and 3.

| number of points | deg = 1 |   | deg = 2 |   | deg = 3 |   |
|------------------|---------|---|---------|---|---------|---|
|                  | Error   | Complexity | Error   | Complexity | Error   | Complexity |
| 3                | 0.00466 | 3           | 0.00465 | 6           | 0.00462 | 10          |
| 4                | 0.00417 | 4           | 0.00416 | 10          | 0.00381 | 20          |
| 5                | 0.00402 | 5           | 0.00399 | 15          | 0.00354 | 35          |
| 6                | 0.00366 | 6           | 0.00366 | 21          | 0.00359 | 56          |
| 8                | 0.00359 | 8           | 0.00359 | 36          | 0.00350 | 120         |
| 10               | 0.00336 | 10          | 0.00325 | 55          | 0.00274 | 220         |
| 12               | 0.00333 | 12          | 0.00322 | 78          | 0.00269 | 364         |
| 18               | 0.00331 | 18          | 0.00318 | 171         | ?        | 1140        |

Table 3. Errors in polynomial regressions depending on the number of previous points. The complexity is the number of parameters.

Here the number of points used for the approximation is larger by 1 than the number of input parameters of the network. The complexity of the network is the number of parameters. For example, the cubic approximation of the brightness of a point by the previous 10 points has 220 parameters (that are coefficients of the corresponding polynomial) and gives error $S = 0.00274$.

To see the error in the original units and before normalization, one takes values of errors $S$ from table 3 and calculate the value of $100 \cdot \sqrt{S}$. For example, for $S = 0.00274$, it is approximately 5.23.

Comparing these with the numbers in table 4 and 5, once sees that, as expected, polynomial regressions work with much less efficiency.

4.3. For comparison: neural networks with some fixed architectures. Here we compare our optimized networks with the networks having some standard architectures. Specifically, we consider a large number of 3-layered networks and maximally fully connected networks. The considered 3-layered networks have from 6 to 20 neurons in the hidden layers, and the considered maximally fully connected networks have up to 500–600 neurons.

The choice of the activation function is a part of the architecture. We consider the most popular ones, and through many computations, choose the one that is the most efficient.
The following activation functions were considered (see their graphs on section 4.3).

- $f_0(x) = x$
- $f_1(x) = \begin{cases} 0, & x < 0 \\ x, & x \geq 0 \end{cases}$ (ReLU)
- $f_2(x) = \frac{1}{1 + e^{-x}}$ (sigmoid)
- $f_3(x) = \begin{cases} -1, & x < 0 \\ +1, & x \geq 0 \end{cases}$ (sign)
- $f_4(x) = 2 \frac{\text{arctan}(x)}{\pi}$
- $f_5(x) = \frac{x}{1 + |x|}$
- $f_6(x) = \text{sign}(x) \frac{x^2}{1 + x^2}$
- $f_7(x) = \text{tanh}(x)$ (hyperbolic tangent)
- $f_8(x) = \begin{cases} x, & |x| \leq 1 \\ \text{sign}(x), & |x| > 1 \end{cases}$
- $f_9(x) = \begin{cases} x/2, & 0 < x \leq 1 \\ (x + 1)/4, & 1 < x < 3 \\ 1, & 3 \geq x \end{cases}$ and then extended using the fact that it is odd.

All but the first three functions are odd. Function $f_6$ was found to be the most effective.

Note that since the minimization process of the neural network is stochastic, repeating the experiment several times, we obtain different results. Thus, for the same architecture, we repeat the experiment 10 times and choose the best result. In fig. 4 are the results of the performance on 5 input points by standard networks.

The envelope from below (the piece-wise linear line) in fig. 4 gives interpolation of our data and allows us to approximate the smallest expected error for a given complexity, or
Figure 4. Complexity and achieved quality (error) for standard networks. The piece-wise linear envelope interpolates the discrete data to give an estimation for the best quality with a given complexity and for the best complexity with a given quality.

vice versa, the lowest complexity for a given error. We use this to compare best achievable results for networks of different complexities. The approach in particular makes sense since the results are of stochastic nature.

We obtained similar results through a large number of experiments with 4 to 12 of the input points for 3-layer and full-connected networks.

4.4. Our algorithm. On the same training matrices, we optimize the architectures using our algorithm.

Table [4] allows us to compare the lowest achievable complexities (for our and the standard networks). For example, in the last line: with 11 input points, among our experiments there is an optimized architecture network with a complexity 128. The corresponding error is 0.00251157. Then the best complexity 312 of the standard networks with the same error is obtained based on the envelope shown in fig. [4]. We see that for the same error, the complexity of the optimized network is significantly less than that of the standard network.

A different type of comparison is given in table [5]. For a given number of points, it shows the best achieved quality (i.e. minimizing $S$) by standard and our optimized networks.

The constructed by our algorithm network architectures can be represented as a graph: neurons correspond to vertices, and connections between neurons correspond to graph
| Number of points | Error          | Best complexity of standard networks for this error | Complexity of optimized networks |
|------------------|----------------|-----------------------------------------------------|----------------------------------|
| 4                | 0.00358090     | 23                                                  | 21                               |
|                  | 0.00345647     | 29                                                  | 22                               |
|                  | 0.00329252     | 61                                                  | 50                               |
|                  | 0.00324596     | 114                                                 | 100                              |
|                  | 0.00323453     | 179                                                 | 119                              |
| 5                | 0.00323960     | 22                                                  | 18                               |
|                  | 0.00290990     | 52                                                  | 50                               |
|                  | 0.00282196     | 329                                                 | 100                              |
| 6                | 0.00316931     | 27                                                  | 21                               |
|                  | 0.00286380     | 56                                                  | 50                               |
|                  | 0.00277786     | 180                                                 | 100                              |
|                  | 0.00276770     | 359                                                 | 118                              |
| 7                | 0.00268228     | 200                                                 | 103                              |
|                  | 0.00266749     | 300                                                 | 116                              |
|                  | 0.00266493     | 374                                                 | 123                              |
| 8                | 0.00266364     | 100                                                 | 66                               |
|                  | 0.00259725     | 162                                                 | 104                              |
| 10               | 0.00263869     | 100                                                 | 67                               |
|                  | 0.00258670     | 150                                                 | 94                               |
|                  | 0.00254739     | 205                                                 | 123                              |
| 11               | 0.00265986     | 100                                                 | 52                               |
|                  | 0.00256666     | 200                                                 | 92                               |
|                  | 0.00251747     | 300                                                 | 121                              |
|                  | 0.00251157     | 312                                                 | 128                              |

Table 4. Comparison of the lowest achieved complexities by our approach and by standard (for the same error).

| number of previous points | standard networks | our optimized networks |
|---------------------------|-------------------|------------------------|
|                           | smallest achieved | corresponding complexity| smallest achieved | corresponding complexity |
|                           | error             |                        | error              |                        |
| 5                         | 0.00323453        | 180                    | 0.003245946        | 78                     |
| 6                         | 0.00282148        | 346                    | 0.002768079        | 415                    |
| 7                         | 0.00276767        | 361                    | 0.002721608        | 339                    |
| 8                         | 0.00266489        | 376                    | 0.002628534        | 261                    |
| 9                         | 0.00257263        | 277                    | 0.00259757         | 101                    |
| 11                        | 0.00252952        | 232                    | 0.002547398        | 124                    |
| 12                        | 0.00251157        | 313                    | 0.002490456        | 173                    |

Table 5. The best results (as measured by the best quality, that is the smallest error) that are achieved in our experiments, for standard and optimized networks.
edges. For better visualization the input values and edges outgoing from these vertices are not shown. Below are a few obtained graphs in “circular” form where vertices of graph are located in the vertices of a regular polygon.

**Figure 5.** 77 weights

**Figure 6.** 120 weights
5. **Comparison with other approaches on image approximation problem**

Here we look into approximating of a black and white graphics file of size $512 \times 512$ by a function of two input variables, $f(x, y)$. We consider 3-layered architectures with two inputs, $N_1$ neurons in the first layer, $N_2$ neurons in the second layer, and 1 output neuron. Here $4 \leq N_1, N_2 \leq 40$. We run the learning process on TensorFlow/Keras. We optimize
these networks using our approach. On fig. 10 is the graph of one of the optimized by us networks.

A comparison of the described networks one can see in table 6. To compare complexities
we use the same approach as in Sec. 4, i.e. construct an envelope from the below to
eextrapolate discrete data that we get from computations, see fig. 9. One can see that for
the same error, our optimized networks offer significantly smaller complexities.

![Graph of one of the optimized networks](image)

**Figure 9.** Blue points are the obtained complexities/errors by the standard networks. The red curve is the envelope of this data extrapolating the obtained results and allowing the comparison for others complexities/errors.

6. Conclusions

We propose a new kind of automatic architecture search algorithm. The algorithm
alternates pruning connections and adding neurons, and it does not restrict itself to
layered networks only. Instead, we search for an architecture among arbitrary oriented
graph with some weights (along with some biases and an activation function), so there
may be no layered structure in such a network. The goal is to minimize the complexity
staying within a given error.

We begin with any standard architecture and create our optimized one by pruning and
letting it grow, pruning and again letting it grow, and so on.

For large networks, where the number of connections counts in hundreds, the complexity
of the optimized network is $2 - 2.5$ times smaller than that of a standard network with
the same error. For small networks, where the number of connections counts in tens, the
Figure 10. The graph of one of the optimized networks. Specific parameters are as follows: 43 neurons (including 2 input neurons), complexity is 503, error 0.004607364. Arrows go from right to left, from vertices labeled with large numbers to vertices labeled with smaller numbers.

complexity decreases by a factor of $1.25 - 2$. Here by standard networks, we mean the best results obtained with 3-layer and full-connection networks.

The algorithm can be sped up by for example not considering every connection while pruning.

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| Given error | Best complexity of standard architectures | Best complexity of our optimized networks |
|-------------|------------------------------------------|------------------------------------------|
| 0.014       | 67                                       | 48                                       |
| 0.013       | 87                                       | 63                                       |
| 0.011       | 117                                      | 99                                       |
| 0.010       | 123                                      | 118                                      |
| 0.009       | 145                                      | 138                                      |
| 0.008       | 182                                      | 169                                      |
| 0.007       | 237                                      | 214                                      |
| 0.006       | 308                                      | 292                                      |
| 0.005       | 408                                      | 371                                      |
| 0.0045      | 474                                      | 410                                      |
| 0.0040      | 590                                      | 449                                      |
| 0.0035      | 768                                      | 488                                      |
| 0.0030      | 987                                      | 527                                      |
| 0.00225     | 1765                                     | 562                                      |
| 0.0020      | —                                        | 606                                      |
| 0.0012      | —                                        | 847                                      |
| 0.0010      | —                                        | 921                                      |
| 0.0007      | —                                        | 1158                                     |
| 0.0006138   | —                                        | 1274                                     |

Table 6. Comparing best complexities achieving the given errors.

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