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Evolutionary Training of Autoencoders by Differential Evolution

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***Abstract*-** In this paper, the author experimentally evaluates the ability of Differential Evolution (DE) algorithm in evolutionary training of autoencoders. DE is an instance of evolutionary algorithms. An autoencoder is a component of a deep neural network known as a stacked autoencoder. Optimization of neural networks by means of evolutionary algorithms is called neuroevolution. Weights and biases in an autoencoder are optimized by DE so that the autoencoder can precisely reconstruct its input data. A dataset of handwritten digits is used in the experiment. The result showed that DE could evolve autoencoders that reconstructed the training and test data well. The result is then compared with previous experimental results by Evolution Strategy (ES), Genetic Algorithm (GA) and Particle Swarm Optimization (PSO), in order to investigate whether DE is better than those three algorithms on the task. The comparison revealed that DE could train autoencoders significantly better than GA, but not significantly better than either PSO or ES. Training error curves illustrated the efficiency of DE in finding good solutions. DE could make the error smaller than 8% much earlier than PSO, ES and GA.

***Keywords*-** *Neural Network, Autoencoder, Evolutionary Algorithm, Optimization*

I. INTRODUCTION

Deep neural networks and their learning algorithms have been actively researched recently [1-14]. A stacked autoencoder is a kind of the deep neural network, where an autoencoder is a kind of layered feed forward neural networks [1,7,8]. An autoencoder can be trained by the well-known back propagation (BP) algorithm [15], but the training of neural networks by the BP algorithm is likely to get stuck in an undesirable local minimum because the algorithm is based on a gradient decent method. Besides, several methods are proposed for training neural networks by using evolutionary algorithms, known as neuroevolution and evolutionary neural networks [16,17]. An advantage of evolutionary algorithms over the BP in training neural networks is that evolutionary algorithms can globally search solutions well and thus the trained neural networks are less likely to get stuck in an undesirable local minimum [18-23]. Therefore, we can expect that evolutionary algorithms contribute well to the training of autoencoders (and thus stacked autoencoders).

The author previously reported experimental results by Genetic Algorithm (GA) [24], Evolution Strategy (ES) [25] and Particle Swarm Optimization [26]. It is known as the "no free lunch" theorem that no single search method is able to find a better solution than any other method does [27]. Thus, various evolutionary methods should be compared for investigating which method suits better and why. As an alternative, Differential Evolution (DE) [28] is adopted in this paper. This paper reports an experimental result by DE, and compares it with the previously reported results by GA, ES and PSO. The same dataset of handwritten digits is consistently used in these experiments.

II. AUTOENCODER

An autoencoder [1,7,8] is a layered feed forward neural network where the number of units in the output layer is the same as that in the input layer. An autoencoder is trained to output the same values as input values, in other words, to reproduce their input data. Fig. 1 shows the topology of an autoencoder adopted in this research. It has a single hidden layer. Usually, the number of hidden units is smaller than those of input (output) layer: N dimensional input real vectors are encoded (compressed) to $M\,(<N)$ dimensional real vectors between the input and hidden layers, and the M dimensional real vectors are decoded (decompressed) to the N dimensional real vectors between the hidden and output layers. Note that the compression/decompression process is not lossless but lossy so that the output vectors are not exactly be the same as the input vectors. An autoencoder is trained to make the error between the input and output vectors smaller.

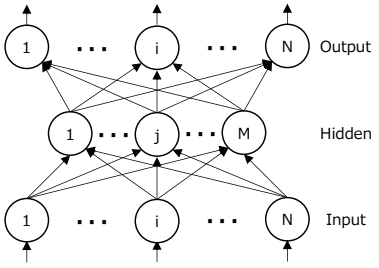

Figure 1. Topology of an autoencoder in this research.

The feed forward calculations in this autoencoder are the same as those in the traditional three layered perceptron. The following equations (1)-(5) show the calculations.

Input layer:

$$out_i^{(1)} = x_i, i = 1,2,\dots,N \quad (1)$$

Hidden layer:

$$in_j^{(2)} = \theta_j^{(2)} + \sum_i w_{i,j}^{(2)}\, out_i^{(1)}, j = 1,2,\dots,M \quad (2)$$

$$out_j^{(2)} = f(in_j^{(2)}), j = 1,2,\dots,M \quad (3)$$

Output layer:

$$in_i^{(3)} = \theta_i^{(3)} + \sum_j w_{j,i}^{(3)}\, out_j^{(2)}, i = 1,2,\dots,N \quad (4)$$

$$out_i^{(3)} = f(in_i^{(3)}), i = 1,2,\dots,N \quad (5)$$

The symbols in (1)-(5) denote as follows:

x_i	Input value to i-th input unit.
$out_i^{(1)}$	Output value from i-th input unit.
$in_j^{(2)}$	Input value to j-th hidden unit.
$w_{i,j}^{(2)}$	Weight value from i-th input unit to j-th hidden unit.
$\theta_j^{(2)}$	Bias value of j-th hidden unit.
$out_j^{(2)}$	Output value from j-th hidden unit.
$in_i^{(3)}$	Input value to i-th output unit.
$w_{j,i}^{(3)}$	Weight value from j-th hidden unit to i-th output unit.
$\theta_i^{(3)}$	Bias value of i-th output unit.
$out_i^{(3)}$	Output value from i-th output unit.

$f()$ is a unit activation function, where the sigmoidal one is adopted in this research: $f(x) = 1/(1+e^{-x})$.

Suppose the training data are *N* dimensional real vectors and the number of the data is D.

$$\boldsymbol{X} = \{\boldsymbol{x}_d\}, d = 1,2,\dots,D \quad (6)$$

$$\boldsymbol{x}_d = (x_{d,1}, x_{d,2}, \dots, x_{d,N}) \quad (7)$$

In (6), $\boldsymbol{X}$ is the set of training data. Each $\boldsymbol{x}_d$ in (7) is the *N*-dimensional real vector. An autoencoder is trained (i.e., values of $w_{i,j}^{(2)}$, $\theta_j^{(2)}$, $w_{j,i}^{(3)}$, and $\theta_i^{(3)}$ are optimized) so that its output values ($out_i^{(3)}, i = 1,2,\dots,N$) become closer to its input values ($x_{d,i}, i = 1,2,\dots,N$). In other words, the input value $x_{d,i}$ is the target for the output value $out_i^{(3)}$. Thus, the error between $x_{d,i}$ and $out_i^{(3)}$ becomes smaller by optimizing the value of weights and biases.

$$e_d = \frac{1}{N}\sum_{i=1}^{N}(out_i^{(3)} - x_{d,i})^2 \quad (8)$$

$$e = \frac{1}{D}\sum_{d=1}^{D} e_d \quad (9)$$

e_d in (8) denotes the error for $\boldsymbol{x}_d$ ($0\% \le e_d \le 100\%$), and *e* in (9) denotes the average error over the entire training data $\boldsymbol{X}$ ($0\% \le e \le 100\%$).

III. Evolutionary Training by Differential Evolution

Instead of the BP, DE is adopted as a training method of the autoencoder in this research. DE is an instance of evolutionary algorithms. Evolutionary algorithms are population-based stochastic search algorithms, whereas the BP is a gradient-based single-point search algorithm. Because of this difference, evolutionary algorithms are better than the BP in searching solutions globally. It was reported that evolutionary algorithms could optimize neural networks better than the BP could [18-23].

Optimization of neural networks by means of evolutionary algorithms is called neuroevolution [16,17]. There are two types of neuroevolution methods: (A) the topology of a neural network (e.g., the number of hidden layers, the number of units in each hidden layer) is fixed and the weights are optimized, or (B) both of the topology and the weights are optimized. In this paper, the author adopts the former method. The autoencoder with the topology shown in Fig. 1 includes $2MN$ ($= MN + MN$) weights and $M + N$ biases. Thus, the autoencoder includes $2MN + M + N$ parameters in total. Let us denote $S = 2MN + M + N$. These parameters forms an S dimensional real vector, $\boldsymbol{y} = (y_1, y_2, \dots, y_S)$, and the vector is treated as the genotype in an evolutionary/swarm algorithm. The phenotype in the algorithm is the autoencoder in Fig. 1. Evolutionary operators are applied to optimize $\boldsymbol{y}$ so that the error becomes smaller. The error value *e* in (9) is calculated with the training data and the output values of an autoencoder.

The process of training neural networks by DE is as follows in this paper:

Step1: Initialization
Step2: Evaluation
Step3: Conditional Termination
Step4: Reproduction
Step5: Evaluation
Step6: Selection
Step7: Goto Step3

In Step1, $\boldsymbol{y}^1, \boldsymbol{y}^2, \dots, \boldsymbol{y}^\lambda$ are initialized as random values, where λ denotes the population size. $\boldsymbol{y}^k$ denotes the genotype vector of the *k*-th parent in the population, i.e., $\boldsymbol{y}^k = (y_1^k, y_2^k, \dots, y_S^k), k = 1,2,\dots,\lambda$. Population size λ is given. The domain range of each genotype value should be neither too large nor too small in this research because the value is used as a weight or bias value in a neural network.

In Step 2, fitness of each parent $\boldsymbol{y}^k, k = 1,2,\dots,\lambda$ is evaluated. In this research, the fitness is based on the error in (9). A parent with a smaller error fits better. In Step 3, the loop of evolutionary process is finished if a given termination condition is met. In this research, the loop is finished if the loop counter reaches to a given number.

In Step 4, new λ offsprings are created by applying the crossover operator to the parents and *donors*. The donors are created before the crossover. The reproduction method called "DE/rand/1/bin" is adopted here. $\boldsymbol{v}^k$ denotes the genotype

vectors of the k-th donor. $\boldsymbol{v}^k = (v_1^k, v_2^k, \ldots, v_S^k),\ k = 1,2,\ldots,\lambda$. $\boldsymbol{v}^k$ is determined as follows.

1. From the λ parents $(\boldsymbol{y}^1, \boldsymbol{y}^2, \ldots, \boldsymbol{y}^\lambda)$ three parents $\boldsymbol{y}^a, \boldsymbol{y}^b, \boldsymbol{y}^c$ are randomly selected where $a \neq \mathrm{b} \neq \mathrm{c} \neq k$.
2. $v_i^k = y_i^a + F(y_i^b - y_i^c), i = 1,2,\ldots,S,$ where F is a preset scaling factor.

$\boldsymbol{z}^k$ denotes the genotype vectors of the k-th offspring. $\boldsymbol{z}^k = (z_1^k, z_2^k, \ldots, z_S^k),\ k = 1,2,\ldots,\lambda$. $\boldsymbol{z}^k$ is determined as follows. $z_j^k = v_j^k\ if\ r < CR\ or\ j = R,$ else $z_j^k = y_j^k,\quad j = 1,2,\ldots,S,$ where r is a uniform random rumber, $0 \leq r \leq 1$, CR is a preset crossover rate, $0 \leq CR \leq 1$, and R is a uniform random integer, $R \in \{1,2,\ldots,S\}$. r is sampled for each $j = 1,2,\ldots,S$, and R is sampled for each $k = 1,2,\ldots,\lambda$.

In Step 5, fitness of each offspring $\boldsymbol{z}^k, k = 1,2,\ldots,\lambda$ is evaluated in the same manner as each parent $\boldsymbol{y}^k, k = 1,2,\ldots,\lambda$. In Step6, the better of parent $\boldsymbol{y}^k$ or offspring $\boldsymbol{z}^k$ is selected as a new parent $\boldsymbol{y}^k$, $k = 1,2,\ldots,\lambda$.

IV. Experiment

This section reports an experimental study in which a dataset of handwritten digits is used as training data. The dataset is the Optical Recognition of Handwritten Digits Data Set which is available in the UC Irvine Machine Learning Repository. [29]

For each of the 10 digits (0,1,…,9), 20 samples are randomly extracted from the data file `optdigits.tra`. Thus, the total number of the sampled data is $10 \times 20 = 200$. A half of the 200 data is used as the training data, and the remaining half is used as the test data. Each data consists of $8 \times 8 = 64$ pixels and a pixel is valued with either of 0,1,…,16 (0: white, 16: black). In this experiment, the pixel values are normalized to a real value within the interval $[0.0, 1.0]$ by dividing the values by 16.0. Figs. 2 and 3 visually show the training and test data respectively.

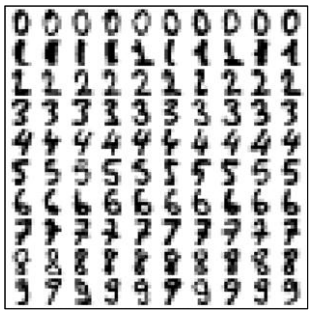

Figure 2. Training data in this experiment

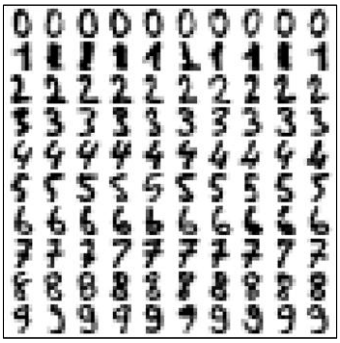

Figure 3. Test data in this experiment

The numbers of units in the input and output layers are 64, because each training data consists of 64 values. The number of hidden units is set to 32, i.e., 50% of the input/output units. Thus, in this experiment, an autoencoder has 64×32+32×64 weights and 32+64 biases in total, and the genotype is a 4192 dimensional real vector.

Parameter values of DE are experimentally set as follows:

- Population size λ: 100.
- Limit of generations: 10,000.
- Number of evaluations: 100×10,000 = 1,000,000
- Genotype values: within the interval $[-5.0, 5.0]$.
- Initial genotype values: randomly sampled from the standard normal distribution $N(0,1)$.
- Scaling factor $F = 0.1$.
- Crossover rate $CR = 0.5$.

The values of error e in (9) were observed for 10 runs. Table 1(a) shows the best (smallest), the worst (largest), and the average of the 10 training error values. Fig. 4 shows the outputs by the trained autoencoder with the best error of 7.78%. The trained autoencoder reconstructs each of the 100 input digits in Fig. 2 to the corresponding output digit in Fig. 4 (the error between the corresponding input/output digits is 7.78% per pixel in average).

If the trained autoencoders overfit to the training data, the training error becomes small but the test error becomes much larger. Table 1(b) shows the test errors, where the test data (Fig. 3) are input to the 10 trained autoencoders. The best one of the 10 trained autoencoders reconstructs each of the 100 input digits in Fig. 3 to the corresponding output digit in Fig. 5, where the error between the corresponding input/output digits is 10.99% per pixel in average. Table 1 reveals that the test errors are larger than the training errors but the differences are small. Thus, DE did not make autoencoders overfit to the training data.

TABLE I. TRAINING AND TEST ERROS (%) BY DE.

	(a) training			(b) test		
	best	worst	average	best	worst	average
DE	7.78	10.44	8.99	10.99	12.32	11.43

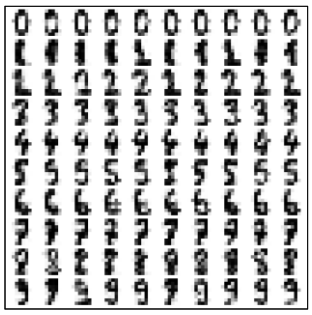

Figure 4. Output digits by the best autoencoder (reconstruction of input digits in Fig. 2)

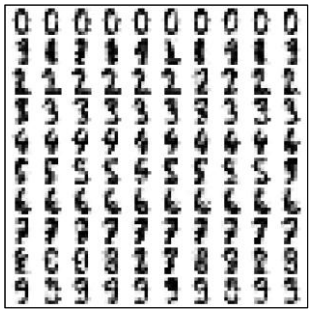

Figure 5. Output digits by the best autoencoder (reconstruction of input digits in Fig. 3)

The author next compares the result by DE with those by other algorithms, ES, GA and PSO, in order to investigate whether DE is better than those algorithms on this task. The author previously reported experimental results by the three algorithms [24-26], where the same training and test data were adopted. In the same manner described in this paper for DE, each of the three algorithms was applied to evolutionary training of autoencoders. The values of error e in (9) were observed for 10 runs with each algorithm. Table 2 shows the training and test errors in the same manner as in table 1. Firstly, the average training error by DE (8.99%) is smaller than the corresponding errors by ES (9.07%) and GA (9.67%), but is larger than the corresponding error by PSO (8.69%). Secondly, the average test error by DE (11.43%) is smaller than the corresponding error by GA (12.63%), but is larger than the corresponding errors by ES (11.23%) and PSO (11.18%). The differences of training/test errors are statistically tested by Wilcoxon rank-sum test.

- The training errors by DE were significantly smaller than those by GA (p=0.03151), but they were not significantly smaller than those by either ES (p=0.5147) or PSO (p=0.7821).
- The test errors by DE were significantly smaller than those by GA ($p=2.436\times 10^{-4}$), but they were not significantly smaller than those by either ES (p=0.8601) or PSO (p=0.7594).

Thus, DE could train significantly better than GA but not than either ES or PSO.

TABLE II. TRAINING AND TEST ERROS (%) BY PSO, ES AND GA [26].

	(a) training			(b) test		
	best	worst	average	best	worst	average
PSO	7.87	9.31	8.69	10.55	11.65	11.18
ES	8.26	10.50	9.07	10.43	12.50	11.23
GA	8.42	11.34	9.67	11.54	13.93	12.63

Fig. 6 illustrates the training error curves along with the progress of evolutionary training (the number of evaluations). Each curve shows errors in the best run among the 10 runs by each algorithm.

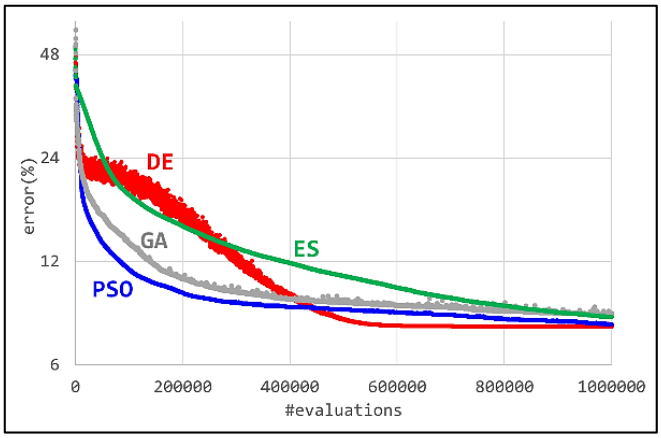

Figure 6. Training errors by DE, PSO, ES and GA.

Fig. 6 revealed that,

- From 100,000 to 200,000 evaluations, the error by DE was the largest, but,
- From 200,000 to 500,000 evaluations, the error by DE decreased more quickly, and
- At 600,000 evaluations, the error by DE reached to a small value which PSO could reach at 1,000,000 evaluations.

Thus, in the early stage, DE explored solutions more globally than the other algorithms, and then DE could exploit solutions more efficiently. This result shows the better ability of DE in balancing explorations and exploitations. This ability stems from the differential vector $\boldsymbol{y}^b - \boldsymbol{y}^c$ in producing the donor $\boldsymbol{v}^k$. In the early stage, the parents $\boldsymbol{y}^1, \boldsymbol{y}^2, \ldots, \boldsymbol{y}^\lambda$ are scattered in the search space so that the differential vector

becomes larger. Therefore, the distance between the parent $\boldsymbol{y}^k$ and the offspring $\boldsymbol{z}^k$ is also larger. Reversely, in the later stage, the parents $\boldsymbol{y}^1, \boldsymbol{y}^2, \ldots, \boldsymbol{y}^\lambda$ are gathered in smaller areas so that the differential vector becomes smaller. Therefore, the distance between the parent $\boldsymbol{y}^k$ and the offspring $\boldsymbol{z}^k$ is also smaller. The idea of adopting differential vectors to the reproduction makes DE a promising algorithm.

V. Conclusion and Future Work

The author adopted DE to the evolutionary training of an autoencoder. The experimental result with the data of handwritten digits showed that DE contributed significantly better than GA but not significantly better than PSO and ES. The error curves illustrated the efficiency in finding good solutions. DE could make the error smaller than 8% much earlier than PSO, ES and GA.

The author will further evaluate, compare and improve the abilities of other evolutionary/swarm algorithms and their hybrids in the training of deep neural networks.

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