

Biologically Inspired Computing

-

Training an Artificial Neural Network using Particle Swarm Optimisation

-

<https://www2.macs.hw.ac.uk/~sf52/Bio-Comp-docs/html/index.html>

Sam Fay-Hunt — sf52@hw.ac.uk
Kamil Szymczak — ks83@hw.ac.uk

November 23, 2020

Contents

1	Introduction	1
2	Development Rationale	2
3	Experimentation Methodology	3
4	Results	4
5	Conclusion	5
5.1	Further work	5
5.2	Discussion	5
A	References	7
B	Additional Material	8
B.1	PSO configuration vectors	8
B.2	ANN configuration vectors	9

1 Introduction

This report details our rationale when developing our Artificial Neural Network (ANN) and Particle Swarm Optimisation (PSO) implementations, A description of the methodology we employed, and the results from the experiments we performed to gain insight into the factors that can effect the quality of PSO.

Our solution is written in Python, heavily utilising numpy, pandas and the python standard libraries, additionally we made use of matplotlib for plotting graphs and SKlearn to split the data into training and testing sets. We used an OOP approach to keep the project organised so we could maintain the fairly large codebase, while keeping the ANN and the PSO modules neatly decoupled. We used jupyter notebooks to demonstrate how to use our codebase, and to present our findings. We used sphinx to generate documentation of the sourcecode, links to our documentation are included throughout this report to help provide context.

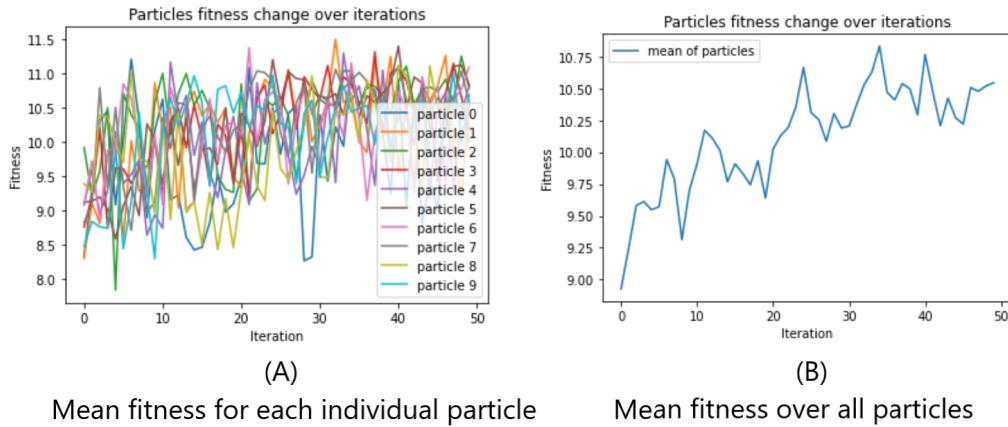


Figure 1: Learning PSO hyperparameters with PSO for the complex dataset.

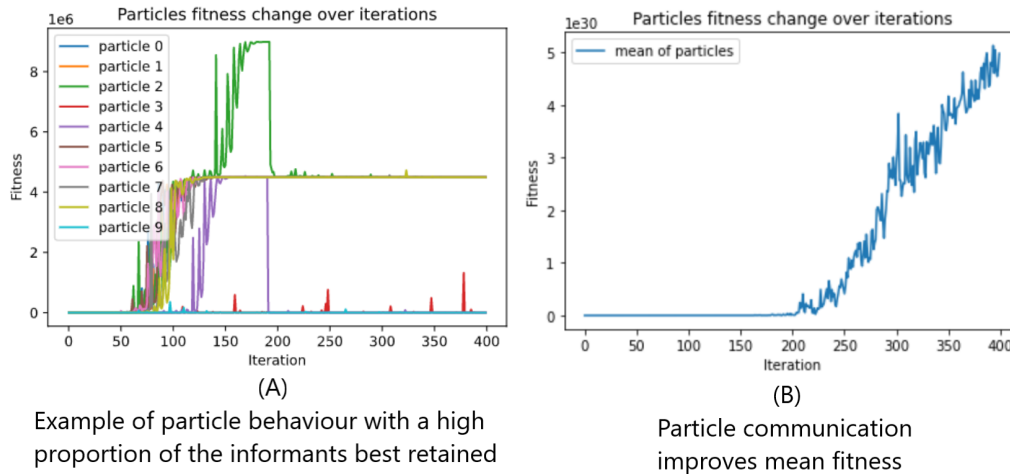


Figure 2: Notable examples of PSO hyperparameters effecting fitness

2 Development Rationale

Our rationale was to create 2 submodules: ANNModel and PSO that could be used to build a fully connected neural network or perform PSO independently. We wanted the submodules to be completely decoupled to allow PSO to work on arbitrary Optimisation problems.

ANNModel is only able to create a fully connected neural network, we made this decision to simplify the process of vectorizing the parameters of the network for optimisation with PSO, this also made converting the vector back into a model easier.

The ANNModel's design was inspired by TensorFlow & Keras (Keras 2020; Tensorflow 2020), specifically when defining the shape of the neural network. For example you can instantiate the empty network, define the input and result vectors, the layers and then, finally, compile the model. Once compiled you can perform a single pass on the model with either random weights or activations, biases and weights defined by a vector.

To develop PSO we used the pseudocode from (Luke 2013), the PSO class utilises a Particle class to abstract away some complexity. To use the PSO class define the hyperparameters in the constructor (as described in the documentation), and then specify the fitness function and search dimensions for PSO.

We created an interface for PSO Called Optimisable, any class that properly implements this interface can be used with our PSO implementation. The beauty of this technique is that it allowed us to implement this interface on our PSO class and construct a (PSO) optimiser for our PSO hyperparameters for a specific model shape, for clarity we refer to this outer PSO optimiser as "meta-PSO" and the inner PSO optimiser as "inner-PSO".

This interface also allowed us to create some wrapper classes(PSOHistory, PSOFittest) that can store detailed data about all the hyperparameter settings of the model being optimised. Figure 3 shows the definitions of the hyperparameters and boundaries that our meta PSO algorithm searches over.

```
def dimension_vec(self):
    swarm_size = (10, 100)
    informants = (4, 8)
    alpha = (0.01, 2.0)
    beta = (0.01, 2.0)
    gamma = (0.01, 2.0)
    delta = (0.01, 2.0)
    epsilon = (0.01, 2.0)
    return [swarm_size, informants, alpha, beta, gamma, delta, epsilon]
```

Figure 3: A list describing the dimensions and boundaries that PSO will search over. See the documentation for more information (Fay-Hunt and Szymczak 2020).

3 Experimentation Methodology

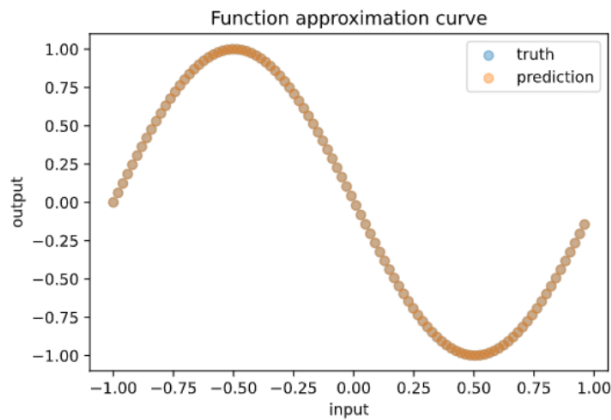
As explained in the previous section, we used a method to find good PSO hyperparameters by applying PSO to another PSO that itself tries to optimize our ANN for a defined dataset. This allowed us to investigate a wide search space of potential optimal hyperparameters for the PSO model that was used to optimize the given ANN.

We ran all experiments defined in Table 1 on a neural network with only 4 neurons in its hidden layer and 1 neuron in the output layer, while this did make it harder to find the ideal neural network hyperparameters for some functions in some cases the results were surprisingly accurate. We used mean squared error as the loss function, also we initialise our ANN with activation functions however the activation functions used are learned by PSO.

To score the hyperparameters we used a subset of the input data from the and calculated the percentage of correct approximations within a tolerance of ± 0.03 .

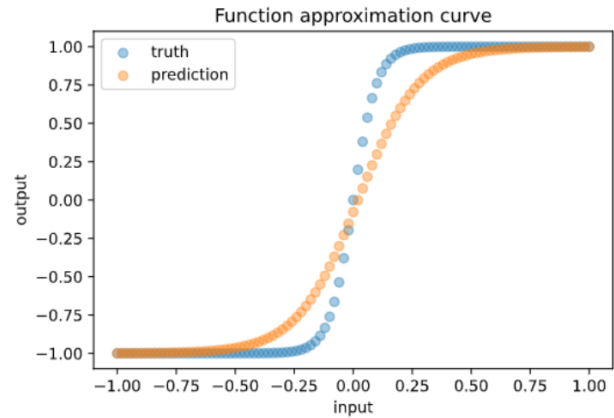
Experiment steps:

1. Run the Meta_pso notebook with each dataset and record the resulting vectors representing the ANN & PSO hyperparameters.
2. Copy the vectors from Meta_pso to the evaluation notebook (See Appendix B.1 & Appendix B.2).
3. For each pair of datasets and corresponding vectors from Meta_pso set the corresponding training/testing data, the decimal places to compare, the PSO, and ANN parameters.
4. Run the tests and record the results.



(A)

Sine approximation



(B)

Tanh approximation

Figure 4: Visualized function approximation curve

(A) is with an improved neural network architecture, (B) is produced by the network defined in Section 3

4 Results

	Experiment	Data	Fitness	Loss	Score*
Cubic	Best ANN Params meta-PSO	Train	55	0.018	15%
		Test	70	0.014	15%
	Best ANN Params (10 runs) mean	Train	46	0.022	28%
		Test	65	0.015	38%
	Average from best PSO params (10 runs)	Train	39	0.026	13%
		Test	50	0.02	11%
Linear	Best ANN Params meta-PSO	Train	10992018104273	0.0	100%
		Test	12840847838954	0.0	100%
	Best ANN Params (10 runs) mean	Train	5.635e+32	0.0	100%
		Test	3.755e+32	0.0	100%
	Average from best PSO params (10 runs)	Train	5.634e+31	0.003	71%
		Test	3.755e31	0.003	69%
Tanh	Best ANN Params meta-PSO	Train	39	0.025	49%
		Test	24	0.041	38%
	Best ANN Params (10 runs) mean	Train	33	0.031	45%
		Test	22	0.046	38%
	Average from best PSO params (10 runs)	Train	25	0.047	32%
		Test	17	0.066	27%
Sine	Best ANN Params meta-PSO	Train	4212	0.0	93%
		Test	24	0.0	88%
	Best ANN Params (10 runs) mean	Train	10.006	0.099	11%
		Test	10.02	0.1	18%
	Average from best PSO params (10 runs)	Train	9.21	0.111	8%
		Test	8.759	0.117	9%
Complex	Best ANN Params meta-PSO	Train	20.17	0.05	9%
		Test	16.05	0.062	18%
	Best ANN Params (10 runs) mean	Train	12.028	0.083	10%
		Test	24.834	0.04	15%
	Average from best PSO params (10 runs)	Train	11.078	0.091	8%
		Test	14.796	0.07	4%
XOR	Best ANN Params meta-PSO	Train	27110227206	0.0	100%
		Test	24306553208	0.0	100%
	Best ANN Params (10 runs) mean	Train	77.32	0.013	100%
		Test	93.254	0.011	100%
	Average from best PSO params (10 runs)	Train	16.716	0.102	95%
		Test	16.023	0.134	88%

Table 1: Table of results, showing the scores from the best ANN parameters from meta-PSO, and the mean best scores from an optimiser using the hyperparameters discovered in meta-PSO.

5 Conclusion

5.1 Further work

Areas for improvement in the experiment:

- We use a fixed model structure for our neural network during testing, so some functions were far easier to approximate than others.
- The fitness function we used was simply $1/\text{loss}$, this was easy to implement but may have impacted the ability of PSO to escape local maximum. In future a alternative fitness functions should be investigated (perhaps one that scales linearly).
- During meta-PSO we only took the mean of 10 inner-PSO runs to evaluate the fitness of each inner-PSO hyperparameter configuration. More would have been better, but impractical in terms of time.

From the experimental results we have observed, we feel future experiments should look closer at other fitness evaluation techniques. An investigation into different hyperparameter search dimensions for both the ANN model and PSO would be interesting, some hyperparameters were found very quickly and it may be worth investigating if we could freeze those once they are found during optimiser runtime and reduce the search dimensions (careful consideration should be made with getting stuck in local maxima here).

A proper benchmark suite should be implemented to identify the serious bottlenecks in computation and memory access so we can begin to address them, and run more comprehensive experiments within a reasonable timeframe. Likewise a unit testing suite would be helpful in identifying any remaining bugs in this codebase, and may also provide some insight into the performance bottlenecks.

Implementing PSO visualization tools to view how the hyperparameters are affecting the fitness in real-time would provide more insight into what is going on with particles during optimization. This information might allow us to identify hyperparameters that tend to result in the particle being caught in local maxima.

5.2 Discussion

The best ANN hyperparameters we observed appeared to be a result of running at least 12.5 million different ANN hyperparameter configurations each time we ran meta-PSO in an attempt to optimise the inner-PSO hyperparameters for a given dataset. This suggests the highest performing ANN hyperparameters discovered during our search for good PSO hyperparameters were more due to reinitialising PSO so many times than actually finding some really good PSO hyperparameters.

Findings in (Garcia-Nieto and Alba 2012; García-Nieto and Alba 2011) indicate that 6 to 8 informants is generally a good number of informants that each particle should have, our own findings support this as seen in Appendix B.1 where the second index in each vector is a float representing the number of informants (when rounded), all have either 6 or 7 informants.

We frequently observed PSO getting stuck in local maxima, this is reflected by the disparity in table 1 between the 10 run mean results and the results recorded from the best

found during meta-PSO. Adjusting the proportion of velocity for each particle to retain and jump size helped to break out of these local maxima but also made the results far more erratic. Meta-PSO found a mean swarm size of 83 particles, this somewhat supports the observation that this is more of a brute force approach by trying many more possible starting points for each PSO we have a higher chance of finding a higher maximum.

We could achieve a significant improvement in fitness, and accuracy in the lower scoring neural networks when we added an appropriate (for the specific function being approximated) number of neurons and layers to the neural network being optimised, however doing so did not guarantee that we would consistently find those optimal ANN hyperparameters. Figure 4 shows a sine function approximation that we found easily with 10 neurons in the hidden layer instead of 4, this had a 100% accuracy score with 0 tolerance to error at 4 decimal places.

A significant factor that prevented more thorough experiments and more comprehensive testing were the performance issues with this implementation, the meta-PSO notebook in some cases would take up to an hour and a half per run even with the extremely conservative settings we chose (See Section 3). When plotting the mean fitness over all particles we could notice an upward trend such as in Figure 1, however any more than 10 particles and 50 iterations was impractical to run. The PSO classes run method in particular has substantial room for improvement, we suspect the performance issues are due to memory access bottlenecks but would need to investigate further to confirm this.

A References

References

- Fay-Hunt, Sam and Kamil Szymczak (2020). *Biologically Inspired Computation Coursework Documentation*. URL: <https://www2.macs.hw.ac.uk/~sf52/Bio-Comp-docs/html/index.html> (visited on 11/22/2020).
- Garcia-Nieto, José and Enrique Alba (July 7, 2012). “Why Six Informants Is Optimal in PSO”. In: *Proceedings of the 14th Annual Conference on Genetic and Evolutionary Computation*. GECCO '12. New York, NY, USA: Association for Computing Machinery, pp. 25–32. ISBN: 978-1-4503-1177-9. DOI: 10.1145/2330163.2330168. URL: <https://doi.org/10.1145/2330163.2330168> (visited on 11/21/2020).
- García-Nieto, José and Enrique Alba (Jan. 1, 2011). “Empirical Computation of the Quasi-Optimal Number of Informants in Particle Swarm Optimization”. In: *Genetic and Evolutionary Computation Conference, GECCO'11*, pp. 147–154. DOI: 10.1145/2001576.2001597.
- Keras, team (2020). *Keras Documentation: The Model Class*. URL: <https://keras.io/api/models/model/#model-class> (visited on 11/22/2020).
- Luke, Sean (2013). *Essentials of Metaheuristics: A Set of Undergraduate Lecture Notes*. Second edition, online version 2.0. Morrisville, N.C.: lulu.com. 239 pp. ISBN: 978-1-300-54962-8.
- Tensorflow (2020). *Module: Tf.Keras.Layers — TensorFlow Core v2.3.0*. URL: https://www.tensorflow.org/api_docs/python/tf/keras/layers (visited on 11/22/2020).

B Additional Material

B.1 PSO configuration vectors

```
# Cubic (10 runs) mean fitness: 44.37869624714425
Cubic_pso_config_mean = [91.38785822, 6.52696304, 0.59416449, 0.43559926,
↪ 0.29415449, 1.29923762, 0.73352514]

# Linear (10 runs) mean fintess: 1103190071387.8752
Linear_pso_config_mean = [85.37707185, 6.86909089, 0.51382895, 0.9798064,
↪ 0.12477974, 0.59493009, 0.89702589]

# Tanh (10 runs) mean fitness: 25.520455427936067
Tanh_pso_config_mean = [55.32621771, 7.52578441, 0.12798331, 0.72531664,
↪ 1.08313114, 0.29216353, 1.3627685 ]

# Sine (10 runs) mean fitness: 434
Sine_pso_config_mean = [8.73729926e+01, 7.54895398e+00, 7.33998847e-01,
↪ 7.52228076e-02, 2.92737853e-01, 3.09977124e-01, 8.51531051e-01]

# Complex (10 runs) mean fitness: 12
Complex_pso_config_mean = [82.66312781, 5.85540776, 0.62559032, 0.58225519,
↪ 0.26541185, 1.38181036, 0.6510299 ]

# Xor (10 runs) mean fitness: 2710748526
Xor_pso_config_mean = [96.15250011, 7.08445513, 0.53364588, 0.62468836,
↪ 1.57375821, 1.50229261, 0.17895104]
```

Figure 5: Vectors describing our best PSO configurations for the various datasets

B.2 ANN configuration vectors

Cubic Most fit model: 109.50653486975476

```
Cubic_ann_params = np.array([ 5.3012172, -0.57272851, -0.29479981, 0.80752501,  
    ↪ -0.45059291, -0.37421024, -0.75524689, -0.44855557, 0.89593846,  
    ↪ 0.21242254, 0.65222056, -0.53284427, -0.79926862, -0.79949714,  
    ↪ 0.96237351])
```

Linear Most fit model: 10965948279221.076

```
Linear_ann_params = np.array([ 0.15520314, 0.2222954, 0.47238101, -0.83439247,  
    ↪ -0.27726962, 0.11339216, -0.7816949, -0.79196132, -0.3392678, 0.41548984,  
    ↪ -0.08055252, 0.12817675, -0.71425698, -0.21576561, -0.7553213 ])
```

Tanh Most fit model: 39.38730853575883

```
Tanh_ann_params = np.array([ 0.09854553, 0.39395654, -0.33737974, -0.12358008,  
    ↪ 0.4334227, -0.98235414, -0.99205521, 0.98638961, -0.97515305, 2.33845816,  
    ↪ 0.51783499, -0.96708832, -0.9922467, 0.9696207, -0.99365926])
```

Sine Most fit model: 4212

```
Sine_ann_params = np.array([ 0.26515734, 0.7400037, -0.0499965, 0.32639921,  
    ↪ 0.03951493, 0.93575309, 0.82658881, 0.95566027, 0.89756768, 3.01482873,  
    ↪ -0.62419448, -0.9322514, -0.99330274, -0.85322129, -0.65752741])
```

Complex Most fit model: 15.36

```
Complex_ann_params = np.array([ 5.16794124, -0.50701965, -0.02085653,  
    ↪ -0.67915966, -0.56917589, 0.93068562, 0.25302176, 0.92653444, 0.67209426,  
    ↪ 0.39299595, -0.75832145, -0.44806736, -0.62409455, 2.26094952,  
    ↪ -0.26506833, -0.86461154, 0.31096583, 0.90781783, 0.72454439])
```

Xor Most fit model: 27107485189

```
Xor_ann_params = np.array([-0.13057076, -0.66250843, 0.0122888, -0.4294471,  
    ↪ -0.56088656, 0.76634383, 0.95302873, 0.27348615, 0.86272884, 0.79509781,  
    ↪ 0.80510636, 0.08453014, 0.86190117, 3.37130705, -0.79043449, 0.74686407,  
    ↪ 0.4886179, -0.22842822, 0.69471657])
```

Figure 6: Vectors describing our best ANN configurations for the various datasets