User's Manual for Downloading the Matlab® Computer Scripts: ANN Simulations (Supplementary Material)

Computer server site: http://geosw.ier.unam.mx/GasG-Scripts-ANNs/

D. Pérez-Zárate, E. Santoyo, A. Acevedo-Anicasio, C. García-López, L. Díaz-González (2018) A Novel Approach of Neural Networks for the Prediction of Geothermal Reservoir Temperatures by using the Gas-Phase Composition of Fluids: Part 1 – Methodology and Optimal Architectures. *Computers & Geosciences (Submitted)*.

A simple and quick user guide for running the ANN simulations is here reported. With these purposes, six computer scripts or open codes were written in Matlab® programming language for the evaluation of the ANN simulations.

A standard or academic use license for Matlab® software is required for running all the ANN simulations. Six Matlab® computer scripts or codes are available for downloading from the institutional repository: http://geosw.ier.unam.mx/GasG-Scripts-ANNs/. To install and to run effectively the Matlab® software and the computer scripts or codes, the following hardware specifications are suggested:

• Operating system: Windows 7 Home Premium 64 bits

• Processor: Intel Core i5-2300, 2.80GHz

• RAM memory: 4 GB (minimum requirements)

• Hard Drive: 500 GB (minimum requirements)

Depending on the hardware specifications, the CPU times elapsed during the ANN simulations are shown in the following Table:

Matlab® Computer Scripts or Codes	Geochemical Databases (used)	Number of Computing Iterations	CPU time intervals elapsed for running the ANN simulations (days)
ScriptANN17.m	$WGDB_1$ (n=527)	1,000	2 – 3
ScriptANN18.m	WGDB ₁ (n=527)	1,000	2-3
ScriptANN30.m	WGDB ₂ (n=503)	15,000	10 – 11
ScriptANN31.m	WGDB ₂ (n=503)	15,000	10 – 11
ScriptANN38.m	WGDB ₃ (n=97)	15,000	8 – 10
ScriptANN42.m	WGDB ₃ (n=97)	15,000	8 – 10
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Computer running instructions (A summarized version). After running the computer scripts or codes, a full report containing either the preliminary or final results obtained from the evaluation of ANN architectures for predicting the target or output variable (BHT_{ANN}). The input data used for such purposes is the chemical composition of the gas-phase of geothermal fluids. The report includes the following ANN parameters:

- Number of input data,
- Number of neurons in the hidden layer,
- Number of iterations used for the ANN training,
- The learning rate factor used for the ANN training,
- As evaluation criteria, the following statistical parameters are also reported in each simulation running for evaluating the prediction performance of the ANN:
 - \circ the minimum correlation coefficient (r_{min}) achieved between the BHT_m and BHT_{ANN},
 - o the coefficient of correlation median,
 - \circ the maximum correlation coefficient (r_{max}) reached between BHT_{m} and $BHT_{\text{ANN}},$
 - o the Root Mean Square Error (RMSE) between BHT_m and BHT_{ANN},
 - o the slope (calculated in a regression analysis between BHT_m and BHT_{ANN}),
 - o the intercept (calculated in a regression analysis between BHT_m and BHT_{ANN})
 - the Garson analysis results in terms of the relative contribution (%) of each input variable considered in the ANN simulation, and
 - the iteration number in which the best results are obtained from the ANN simulation.

From these results, a summary of the ANN architectures evaluated for the prediction of reservoir temperature is finally reported (see Tables 8 - 10).

The following pictures are shown to demonstrate the use of the computer scripts or codes in the Matlab® Software environment:

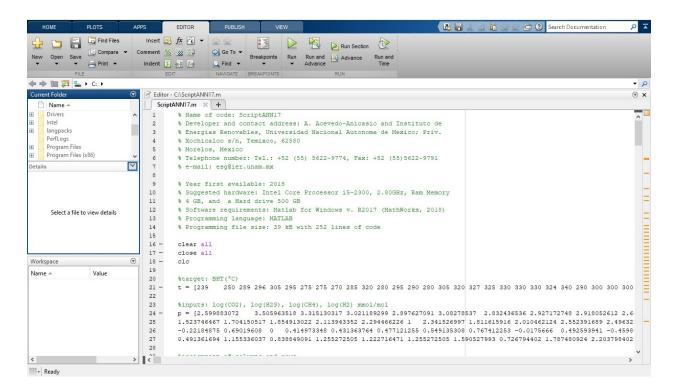


Fig. 1 An example of the uploading process of the ScriptANN17 in the Matlab® computing environment

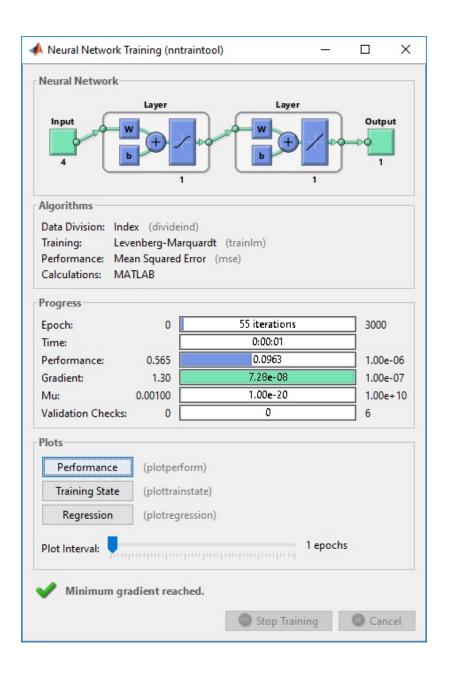


Fig. 2 An example of the Matlab® computer module used for a typical training process of an ANN architecture

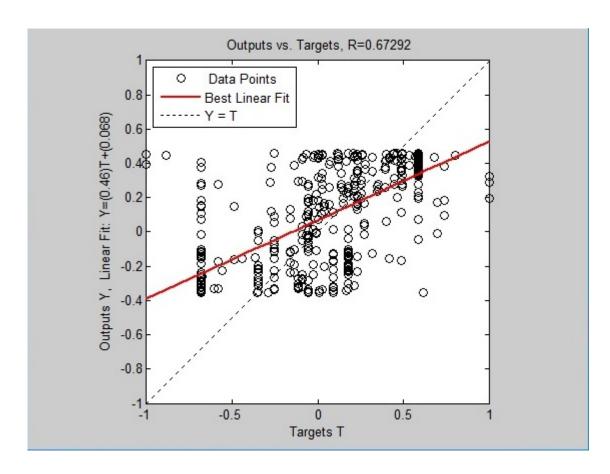


Fig. 3 The preliminary regression analysis between the BHT_m and the simulated BHT_{ANN}

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If some instructions or doubts are still needed from the users, all the authors of the submitted manuscript are available to provide some additional hints for a successful application of the script codes.

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