BRIEF TUTORIAL

The GSA methods is used to fit functions in experimental data. It is based on the correlation between the minimization of a cost function (or objective) obtained through a slow cooling. In this method, an artificial temperature is introduced and gradually cooled in complete analogy with the well known annealing technique, frequently used in metallurgy when a molten metal reaches its crystalline state (global minimum of the thermodynamics energy). In our case the temperature is intended as an external noise.

GSA REQUIRED PARAMETERS:

qA : Acceptance index
qT : Temperature index
qV : Visiting index
To : Initial Temperature
NStopMax is number of parameters used in the function to be optimized.

*Obs.
The *q's* parameters are positive real numbers different of 1, except the qA. The program, initially, present some default parameters.

To parameter: In this procedure, the artificial temperature (To) is introduced and gradually cooled, in complete analogy with the well known annealing technique frequently used in metallurgy when a molten metal reaches its crystalline state (global minimum of the thermodynamical energy). In this case the temperature is intended as an external noise. See the basic references.

FUNCTION:

How to enter the objective function, or cost function, used in the fitting procedure? There are 2 options:

1)- Using the functions included in NumPy scientific package for Python. Examples: np.sin(x), np.exp(x) and others. In this case the 'np.' is mandatory. For additional informations see:
https://www.numpy.org/devdocs/user/quickstart.html

2) Create a user-defined fitting function through the Fitting Function Box. The formatted text fields provide a way for user to introduce the own function as for example: a[0]*x**2 + a[1]*x + a[2] for a quadratic function type.

FUNCTION INITIAL CONSTANTS:

a[i] are the constants used in the function definition as for example the quadratic function f = a[0]*x**2 + a[1]*x + a[2]. x is the independent variable.

Lock: Check box to lock a parameter. In this case, it is not changed during the adjustment procedure.

GRAPHICS OPTIONS:

Animation: The 'Check Boxes' must be activated to show function fitting procedure.

Step Size field: refers to the number of steps in order to update graphic animation.

* Too low values in the ‘StepSize’ will cause the chart updates excessively, which may leave the adjustment slow.

BUTTONS:

Open File: Click in the button to upload the file with input data. The X,Y data must be separated by a single comma in the input file, like in ‘csv’ format.

Fitting: Click to start the fit procedure. The process completes when the difference between reduced chi-square values of two successive iterations is less than a certain tolerance value or when the maximum number of cycles (NStopMax) is reached. When the process completes, we say that the fit has converged.

Save: Click to save final results and additional informations. The Save Dialog can be used to write output file name and to select local to save it.

REFERENCE

Basic reference: Mundim, K. C. and Tsallis, C. Int. J. Quantum Chem. (1996) 58, 373.

For additional information access: www.cursosvirtuais.pro.br/GSA/