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A genetic algorithm to calibrate dynamical systems: Confidence intervals for parameters and residuals

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***Abstract*—This paper presents a genetic algorithm to calibrate dynamical systems that is able to calculate confidence intervals for the parameters of the system. As an application case is used to calibrate the system that reproduces the dynamical response of the General Factor of Personality (GFP) to a given stimulus, particularly to a stimulant drug dose. The model is called in Literature as the *response model* and includes an integro-differential equation. The presented application case is a single case ABC experimental design where the stimulus is methylphenidate.**

***Keywords*-*General Factor of Personality; genetic algorithm; dynamics; integro-differential equation; calibration; methylphenidate*.

1. Introduction

The here presented genetic algorithm has been designed for a particular case but, changing the corresponding system equations it can be used to calibrate any other system. The considered particular case is a system that determines the evolution of the personality of a subject as a consequence of receiving a certain stimulus, for instance a drug dose. In the application case here presented, methylphenidate is the drug being used. It is a powerful psycho-stimulant. This psycho-stimulation can be measured by the *General Factor of Personality* (*GFP*), as a universal observable feature of personality. A questionnaire containing the five adjectives scale that is described by Amigó, Micó & Caselles [3][5] and constructed specifically to assess *GFP* in the context of the *Unique Trait Personality Theory* (*UTPT*) [1][5] is used for the considered case. The *UTPT* claims for a unique trait, as synonymous of single trait, substituted later by the equivalent concept of *GFP*, to represent the overall human personality. The *GFP* is the psychological expression of the activation level of the organism stress system. In fact, in the context of the *UTPT*, *GFP* is called also *extraversion* in a wider sense than the one used in behavioral science, i.e., in the sense of activation level of the organism stress system.

The evolution of the *GFP* is calculated by the *response model* that is an integro-differential equation that has been widely assessed in the context

of different experimental designs. It can reproduce the acute effect of a stimulant drug [2][6][9][10][11]. The model reproduces the dynamical pattern forecasted by Solomon & Corbit [13] and Grossberg [7], by using the hedonic scale, and by Amigó [1] for the *GFP*, i.e., a typical inverted-U.

The here performed calibration of the model is based on a genetic algorithm. Genetic algorithms (*GAs*) are Evolutionary Algorithms (*EAs*) (they adapt their parameters according to previous results) that try to imitate Natural Selection inside a population through parent selection, recombination, mutation and migration. About details on *GAs* and its use in systems calibration, see for instance: Whitley, [14], Guzmán-Cruz et al., [8] and Muraro & Dilao [12]. Nevertheless there are a lot of possible options for their definition, obviously related on how to perform *selection*, *crossover* and *mutation*. The here introduction of *immigration* could be a novelty.

2. The response model

The kinetic part of the response model provides the evolution of the stimulus amount $s(t)$, present in plasma after intake by the individual. It is given by the time function:

$$s(t) = \begin{cases} \frac{\alpha \cdot M}{\beta - \alpha}(exp(-\alpha \cdot t) - exp(-\beta \cdot t)) : \alpha \neq \beta \\ \alpha \cdot M \cdot t \cdot exp(-\alpha \cdot t) : \alpha = \beta \end{cases} \quad (1)$$

Equation (1) is the solution of two coupled differential equations [11], which assumes that no drug/stimulus is present in the organism before consumption. In (1) *M* is the initial amount of a drug single dose, α is the stimulus assimilation rate and β is the stimulus elimination rate. The dynamics of the *GFP* is given by the following integro-differential equation [11]:

$$\left.\begin{array}{c} \frac{dy(t)}{dt} = a\big(b - y(t)\big) + \frac{p}{b}s(t) \\ -b \cdot q \cdot \int_0^t e^{\frac{x-t}{\tau}} \cdot s(x) \cdot y(x)\, dx \\ y(0) = y_0 \end{array}\right\} \quad (2)$$

In (2), *s(t)* represents the stimulus; *y(t)* represents the *GFP* dynamics; and b and y_0 are respectively its tonic level and its initial value. Its dynamics is a balance of three terms, which provide the time derivative of the *GFP*: the *homeostatic control a(b-y(t))*, i.e., the cause of the fast recovering of the tonic level *b*, the *excitation effect p·s(t)/b*, which tends to increase the *GFP*, and the *inhibitor effect* $\int_0^t e^{\frac{x-t}{\tau}} \cdot s(x) \cdot y(x)\, dx$, which tends to decrease the *GFP* and is the cause of a continuously delayed recovering, with the weight $e^{\frac{x-t}{\tau}}$. Parameters *a*, *p*, *q* and τ are named respectively the *homeostatic control power*, the *excitation effect power*, the *inhibitor effect power* and *the inhibitor effect delay*. All the parameters of the model depend on the individual personality or individual biology and on the type of stimulus.

3. The genetic algorithm used for the response model calibration

The program we use for calibration has been ad hoc designed for the previously described model but it can be adapted easily for systems with the following characteristics:

(1) Real data are deterministic. In the case of the *response model*, real *GFP* is measured by the responses of an individual to a questionnaire every some minutes. And model parameters are specific of the individual.
(2) The system to be calibrated is deterministic.
(3) All parameters have a continuous range of possible or plausible values from a maximum to a minimum value.
(4) A single objective variable (function) must be considered, but it may be designed as a weighted combination of several other ones.
(5) Parameter space (search space) is a multidimensional compact space (continuity is assumed in parameter values inside a range of possible or plausible values).
(6) In order to assure the global character of the found optimum three strategies are considered:
    a. A random sample may be analyzed, from the entire search space or from specific zones, in order to identify starting points.
    b. Random migrants with reproduction capacity are introduced inside the current population in every generation.
    c. Several iterations are performed using the previous optimum as a new starting point, up to no improvement is found or the top number of iterations is reached.

3.1. The needed data

The *response mode* has seven parameters: α, β, a, b, p, q, τ and M (M may also be adjusted like the other parameters when the stimulus is not measurable, for instance: a placebo), which meaning has been previously explained. A vector of nine components containing a value for each parameter plus the corresponding *GFP* (y) may be considered as an individual of a population of possible characterizations of the system. The staring values of the parameters (given by previous knowledge), their maximum values, their minimum values, their search window width (% of their initial value), and their search step width (% of their initial value) have to be introduced at the beginning of the search process. Other needed data are the number of experimental values, their time step, and their values. The integration method (Euler or Runge-Kutta-4) and the integration step size have to be also specified. The function to be optimized may be the mean squared deviation (s^2), the determination coefficient (R^2) or the relative mean deviation.

The *GA* may be optionally used, and in the case it is used the following options must be specified: number of individuals of the population, percentage of the population corresponding to reproducers (the best individuals), number of immigrants per generation, mutant genes per thousand in a new individual, number of generations inside a given iteration, and maximum number of iterations. In the case of not using the *GA* but only analyzing a sample, it may be exhaustive or uniformly random. This sampling process also admits iterations.

3.2 The GA pseudo-code

The proposed *GA* intends to be the simplest possible one in order to be as fast as possible without restricting the possibility to find a global optimum. The following pseudo-code might be enough descriptive of the here presented *GA* that we name *PARDOSU*.

```
Introduce data and options
Define the initial population (vectors with random values for parameters and the objective function value)
For i=1 to “number of iterations”, do:
  For j=1 to “number of generations”, do:
    Arrange population from lower to higher the objective function
    Retain the best individuals and eliminate the remaining ones
    Incorporate some immigrants (randomly defined inside parameters’ ranges)
    “Complete the population by reproduction (with mutation) of the present individuals, i.e.:”
    For k=”number of reproducers”+1 to “population size”, do:
      Choose randomly the “father” and the “mother” of the new individual
      For each gen (parameter) choose randomly whether it comes from “father” or “mother”
      For each gen (parameter) choose randomly whether it is newly randomly defined or not
    Next new individual
  Next generation
  If “previous optimum is not improved” Then Exit-Iterations-Loop Else Continue
  Use the optimum individual as new starting point
Next iteration
Calculate residuals by comparing the found optimum with the experimental values
Test residuals for Normality and zero-mean
If “yes” Then “calculate confidence intervals to define the optimal fitting evolution band”
For j=1 to “number of parameters + objective function” do:
  Test parameter j for normality inside the best individuals group
  If p-value for normality is acceptable Then
    Calculate and write the corresponding mean, standard deviation, chi-squared, t of Student and the upper and lower bounds of the confidence interval
    Else write only the corresponding mean, standard deviation and chi-squared
  End If
Next parameter
Write all other results
```

4. The response model calibration

The studied application case consists in one subject that consumed 20 mg of methylphenidate. The Five Adjectives scale questionnaire (adventurous, daring, enthusiastic, merry and bored) was filled out before consumption and after consumption every 15

minutes during 4 hours. The interval of the *GFP* measures is $y \in [0,25]$. The calibration result of the response model for the *GFP* dynamics is provided in Figure 1. With respect to parameters, inside the best individuals group, most of them were not normally distributed (very high chi-squared values), others were constants or with relatively low standard deviations. Note in Figure 1 that it considers the confidence intervals, for a 95% of confidence level, provided by the random variablility values of the parameters.

5. Conclusions

Figure 1 shows the calibration result of the response model for the *GFP* response as a consequence of 20 mg of methylphenidate obtained with the proposed *GA*. The obtained determination coefficient value R^2 supports model applicability as in other studies from literature (see Section 1). The algorithm shows a good performance and time efficiency.

For future work we aim to compare the efficiency of the present features of *PARDOSU* with alternative specific features, such as for instance: mutation of each parameter restricted to values close to the present one, optional equipotency of gens (at present all gens are dominant/recessive), and incest prevention. Options such as selection by competition are discarded due to they do not guarantee the permanence of the best individuals inside the population.

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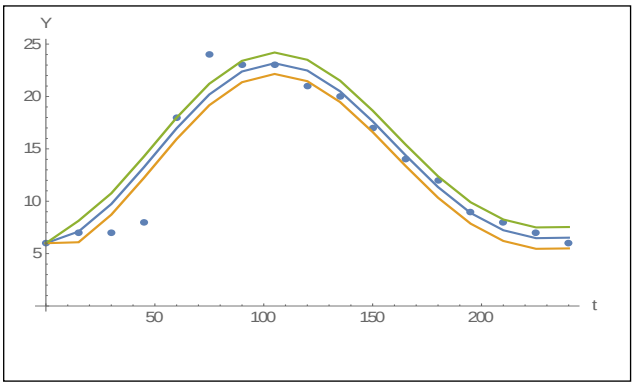

Figure 1: *GFP* (Y) versus time (t). Experimental values (dots) and the calibrated response model (line). R^2=0.92.