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Parameter estimation in mathematical models using the real coded genetic algorithms

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Abstract

In this study, parameter estimation in mathematical models using the real coded genetic algorithms (RCGA) approach is presented. Although the RCGA is similar with the binary coded genetic algorithms (BCGA) in terms of genetic process, it has few advantages such as high precision, non-existence of Hamming's cliff etc., over the BCGA. In this approach, creating initial population and selection procedure are almost the same with the BCGA, but crossover and mutation operations. The proposed approach is implemented on the second order ordinary differential equations modeling the enzyme effusion problem and it is compared with previous approaches. The results indicate that the proposed approach produced better estimated results with respect to previous findings.

Keywords: Real coded genetic algorithms; Binary coded genetic algorithms; Nonlinear curve fitting; Parameter estimation; Ordinary differential equations; Dynamic system identification

1. Introduction

Mathematical models based on a system of ordinary differential equations (ODEs) are widely used in many applications. The solutions of such models can not be expressed by elementary functions in most cases and contain unknown parameters which are usually estimated by experimental data obtained from well-defined standard conditions. This type of problem is usually called parameter estimation in the literature and is often solved by deterministic optimization methods such as Nelder–Mead, Levenberg–Marquardt, Gauss–Newton etc., (Abbasi, 2006; Bayram & Yildiz, 1999; Yildirim, 2003). Unfortunately, the solution to the problem using these methods is usually around the local minima if there are more than one minimum available.

However, better solutions may be found by one of stochastic optimization methods to obtain global minima if they exist in the given search space. The genetic algorithms (GA) method, the best known stochastic optimization technique, imitates the natural evolution process (Coley, 2003; Gen & Cheng, 2000; Goldberg, 2003). One of the main advantages of this method is that it require no gradient of the objective function and additional information. Recently there has been an increasing trend to the real coded GA (RCGA) method for parameter estimation in various applications due to the number of drawbacks of the binary coded GA (BCGA) method. In this study, the RCGA approach is employed for the problem under consideration. The results are considerably improved with respect to previous findings in many aspects such as accuracy, computation time etc.

2. Parameter estimation for dynamic systems

ODEs have been a useful tool for describing the behavior of wide variety of dynamic physical systems since they were numerically solved by using few methods (Chapra & Canale, 2002; Schiling & Harris, 2000). A system of the first order ODEs can be stated by

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$$\frac{dx}{dt} = f(t, x; a), \quad \alpha \leqslant t \leqslant \beta \tag{1}$$

where t, x and a the independent variable which denotes time, the dependent variable or solution which is $n \times 1$ vector called state of the system and a is coefficient-constant parameter vector such as a_1, a_2, $a_3 \ldots a_n$ respectively. If the function f is sufficiently smooth, there is a unique solution of x over the interval $[\alpha, \beta]$.

On the other hand, a slightly complicated dynamic physical system defined by the second order ODE can be given by

$$\frac{d^2x}{dt^2} = f\left(t, x, \frac{dx}{dt}; a\right), \quad \alpha \leqslant t \leqslant \beta \tag{2}$$

where dx/dt is the first derivative of x.

In addition, experimental data set are obtained after m measurements of x against t and we usually assume that $n \ll m$ for the least-square approximation. The problem we meet here is to estimate optimum parameters vector a^* as accurate as possible using the given experimental data. In fact, this is a typical minimization problem which can be defined by

$$E(a) = \sum_{k=1}^{m} w_k [F(t_k; a) - y_k]^2 \tag{3}$$

where w_k is the weight number for the kth data sample if $w_k > 0$ and it is uniform when $w_k = 1$. Besides, $F(t_k; a)$ and y_k are the numeric solution of the mathematical model and experimental data point for kth data point, respectively.

There may be instances where some of the measurements are known to be more accurate and in these cases larger values can be used for those weights but in this estimation, they are assumed to be uniform. The objective here is mainly to find a $n \times 1$ coefficient vector a that minimizes the error.

$$\begin{aligned} &\text{minimize} : E(a) \\ &\text{subject to} : a \in R^n \end{aligned}$$

The function f whose coefficients minimize $E(a)$ is referred to as the weighted least-squares fit or simply the least-squares fit. Although alternative error criteria can be used, the least-squares objective in Eq. (3) is preferred because solution can be easily found.

In this study, we focused on estimation of unknown parameters in the enzyme effusion problem which can be defined by the second order ODE with unknown initial conditions. In this case, there will be the two approaches to identify these initial conditions. The one is to take the first experimental data as an initial value of the model and the other is to predict the initial values as estimated coefficients. Despite the measured data contain experimental error, the least-square approximation to the data $\{(t_k, y_k)\}$ can minimize this error. As a result of this, the former approach was used to estimate the coefficients using the RCGA. The implementation of the RCGA is explained in the following section.

3. Overview of the RCGA method

3.1. Simple genetic algorithms

The GA method is based on a computer simulation of biological evolution and initially works with a randomly generated population consisting of several individuals. A new population is built up by selecting individuals among members of the initial population according to their fitnesses through fundamental genetic process of selection criterion. Once the selection is completed, the crossover operation is put into effect on the new population. Next, the mutation operation is implemented on previous population. Thus, first generation is completed and genetic process is repeated until the termination criteria are satisfied. It should be noted that if the best individual is not the one as desired after completing the genetic process, the advanced operators may be used.

3.2. Selection and reproduction

The reproduction is a process in which individuals in previous population are copied into a mating pool according to their fitnesses. Selecting individuals is carried by a selection criterion such as the roulette wheel, tournament, etc. In this study, the roulette wheel selection which is fitness proportional was employed. The mechanism behind this selection is that an individual with greater fitness value has a greater chance to be copied into the mating pool or vice versa. However, there is no guarantee to copy the fittest individual into the pool in this selection strategy. Therefore, elitism is often used to maintain the best individual for next generation. Average fitness of the current population usually increases after proceeding selection.

3.3. Crossover

The crossover is the most significant operator to generate dissimilar individuals which may be possible solutions to the problem under consideration. Once the new population is formed by selecting individuals among the previous population, crossover operation is put into effect on the current population. Although there are many crossover types such as single point, two points, multi points, uniform, cycle, etc., the former is widely preferable owing to its simplicity. The crossover operation only occurs when its probability is greater or equal to the randomly generated number between 0 and 1. In the real coded crossover used in this algorithm, two individuals are randomly chosen among the population. Fractional numbers of dx and dy are generated by multiplying randomly chosen individuals with a random number between 0 and 1. Thus, new offsprings are created by adding dx and dy to the chosen individuals and this procedure is repeated until the number of crossover offsprings reaches the same size of the parent population. In this research work, crossover probability was 0.60 during all the genetic operations.

3.4. Mutation

Reproduction and crossover make the current population gradually stronger and individuals of the population resemble each other as the genetic process continues. This is expected trend but, if individuals become similar in early generations, the possible solutions will be trapped by local optima due to lack of genetic diversity. Since the reproduction and the crossover operators have no straight forward mechanism to avoid local optima, the mutation operation is proceeded to increase the diversity. The mutation operation only occurs if a randomly generated number between 0 and 1 is less or equal to the mutation probability. When mutation takes place, the current individual is multiplied by a random number between 0 and 1 to produce dx fraction, mutated individual is then obtained by adding dx to current individual. Each individual in the population has a chance to be subjected to mutation even though its probability is very small. In this study, the jump mutation was implemented and its probability was 0.05.

4. Solution of parameter estimation problems

In this parameter estimation problem, unknown parameters and initial conditions aim to be predicted by the RCGA method and cubic spline functions through the experimental data, respectively. For randomly generated each parameter value, the second order ODE is numerically solved by the fourth order Runge–Kutta method, in which the error depending on the step size h is chosen to be a global truncation error of order h^4. Fitness value of ith individual can be calculated by

$$f_i = \frac{1}{E_i(a)} \tag{4}$$

where $E_i(a)$ is the sum of squared error for ith individual. For estimation process, the RCGA method is used to carry out following steps:

I. Create a population with 100 individuals.
II. Evaluate fitness for each individual.
III. Select individuals according to their fitness values and build a temporary population.
IV. Implement single point real crossover with the probability of 0.6 on the temporary population.
V. Mutate the current population with the probability of 0.05.
VI. Repeat steps II, III, IV, V and VI until the number of generation is met.

5. Test functions

Example 1. Mathematical model of enzyme effusion problem (Nyarko & Scitovski, 2004) can be expressed as

$$\frac{\mathrm{d}x_1}{\mathrm{d}t} = a_1(27.8 - x_1) + \frac{a_4}{2.6}(x_2 - x_1) + \frac{4991}{t\sqrt{2\pi}} \exp\left(-0.5\left(\frac{\log(t) - a_2}{a_3}\right)^2\right) \tag{5}$$

$$\frac{\mathrm{d}x_2}{\mathrm{d}t} = \frac{a_4}{2.7}(x_1 - x_2) \tag{6}$$

The software was run to estimate four unknown constant coefficients in the above second order ODE using experimental data given in Table 1 and Eqs. (5) and (6).

Since there are no measured x_2 values, they are numerically solved by setting its initial value to be zero after trials of few attempts. This, of course, affects the solution of the problem, but zero initial value of x_2 is the best among them. Table 2 shows estimated results obtained from solution of the mathematical model. Estimated parameter values, initial values for x_1 and x_2, number of generation and the SSE are comparatively given in Table 2. As the number of generation increases, the SSE slightly increases according to Table 2. Normally, this slight increase can be attributed to stochastic optimization process and it may be ignorable. It is also noted that there

Table 1
Experimental data for enzyme effusion problem (Nyarko & Scitovski, 2004)

t	x_1	t	x_1	t	x_1	t	x_1
0.1	27.8	21.3	331.9	42.4	62.3	81.1	23.5
2.5	20	22.9	243.5	44.4	58.7	91.1	24.8
3.8	23.5	24.9	212	47.9	41.9	101.9	26.1
7	63.6	26.8	164.1	53.1	40.2	115.4	33.3
10.9	267.5	30.1	112.7	59	31.3	138.7	17.8
15	427.8	34.1	88.1	65.1	30	163.2	16.8
18.2	339.7	37.8	76.2	73.1	30.6	186.7	16.8

Table 2
Comparison of estimated parameters with previous estimated results

Method	a_1	a_2	a_3	a_4	x_1 (0.1)	x_2 (0.1)	Generation	SSE
RCGA	0.2624	2.6378	0.3599	0.2212	28.5443	0.2339	100	3068
RCGA	0.271	2.6442	0.3676	0.2429	28.5203	0.2566	500	3120
Nyarko and Scitovski (2004)	0.31938	2.70104	0.3892	0.07819	21	38.75	100	5229
Nyarko and Scitovski (2004)	0.28452	2.67169	0.39268	0.16144	23.99	40.14	500	4068
Khalik (2007)	0.2454	2.6092	0.3326	0.3217	22.005	38.608	100	4432
Khalik (2007)	0.2619	2.6336	0.3524	0.2575	21.986	38.704	300	4137
Scitovski and Jukic (1996)	0.319	2.701	0.419	0.103	22	39	–	5076

is much difference between values of x_2 at 0.1 s because its initial value is set to be zero during numeric solution of the model as mentioned earlier. Besides, the proposed algorithm produces a better result for the solution of the model x_1 at 0.1 s and it can be said that it is very close to the experimental at the same point. The estimated parameters are almost similar with previous findings for the model. For a comparison, variations of the estimated and experimental data with time are shown in Fig. 1.

As seen from Fig. 1, the estimated data closely follows the measured data although there are small differences between them in the certain time ranges. Besides, the rate of change of x_1 exhibits a similar trend with the measured and estimated data at times being larger than 75 s.

Example 2. The analytic solution of mathematical model containing a second order ODE can be stated by

$$y(t;a) = a_1 \exp(a_3 t) + a_2 \exp(a_4 t) \tag{7}$$

where again a_1, a_2, a_3 and a_4 are the unknown parameters.

In this estimation process, the error criterion is the SSE and can be expressed as

$$E(a) = \sum_{k=1}^{m} w_k [a_1 \exp(a_3 t) + a_2 \exp(a_4 t) - y_k]^2 \tag{8}$$

where y_k is the kth experimental data (Khalik, 2007).

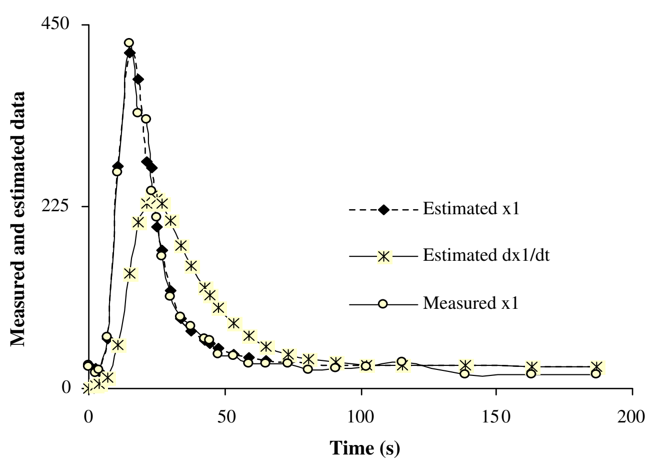

Fig. 1. Variations of estimated and measured data with time for Example 1.

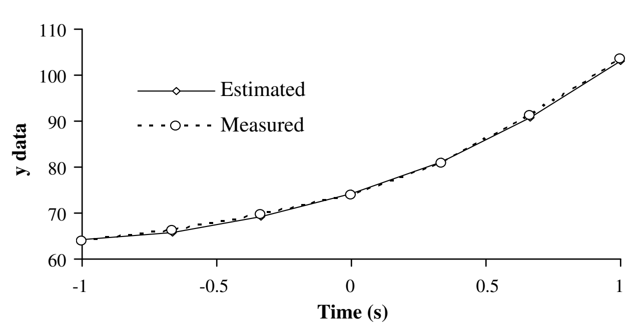

Fig. 2. Variations of estimated and measured data with time for Example 2.

Table 3
Experimental data for Example 2 (Khalik, 2007)

t	64	66	69.5	74	80.8	91	103.5
y	−1	−0.6666667	−0.3333333	0	0.3333333	0.6666667	1

These parameters are aimed to estimate through the measured data using the RCGA and the estimated results are given in Table 3. Fig. 2 shows variations of the estimated parameters and measured data with time. As seen from Fig. 2, the estimated parameters are very close to the measured data in the given range.

6. Conclusion

The results show that the RCGA can be efficiently used to estimate unknown coefficients in the mathematical models containing the second order ODEs. Initial values of the ODEs are highly influential on the numerical solution of the model in this estimation process as expected. To minimize computation time in function evaluation, the fourth order Runge–Kutta method can be employed and it is as accurate as the Runge–Kutta–Fehlberg method for the same application. In mathematical models where no initial values are given, the cubic spline functions can be used to obtain them from the experimental data. This can help increase the estimation performance in finding improved parameter values. The number of generation is not very influential on obtaining more improved estimated parameters but population size, crossover and mutation rates.

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