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Proceedings of the 5th International Conference on Inverse Problems in Engineering: Theory and Practice, Cambridge, UK, 11-15th July 2005

RETRIEVING OSCILLATORY SOLUTIONS FROM SYSTEMS OF DIFFERENCE EQUATIONS

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Abstract - The inverse problem relating to the field of complex oscillatory dynamics mathematical modeling has been formulated and analyzed. A robust method for retrieving and classifying oscillatory solutions of systems of difference equations is proposed. The method is based on a genetic algorithm with a special type of fitness function. An example is presented of retrieval of complex oscillations embedded in difference equations derived from the discrete chaotic dynamics of physicochemical reactions.

1. INTRODUCTION

Mathematical models in the form of nonlinear difference equations are widely used to simulate the dynamics of complex systems, including oscillatory chemical reactions, internal human rhythms revealed by electrocardiograms and electroencephalograms, socio-economic systems, and other systems [8, 12]. It is well known that the dynamics of such systems exhibit complex periodic and chaotic oscillations. The construction and solution of the systems of non-linear difference equations for mathematical modeling of complex systems with chaotic behavior will be termed the forward problem. In the work presented here, we sought to use the specific types of difference equations resulting from physicochemical reactions discrete chaotic dynamics [6-9] as the mathematical model.

Discrete chaotic dynamics (DCD), a theory based on first physical principles, leads to basic equations in the form of systems of difference equations. A specific type of system of difference equations is constructed for each particular multicomponent system, reflecting the mechanism of internal interactions between the system's constituents (agents) accomplished with "information exchange". Systems of difference equations derived from DCD are known to be a source for the various types of complex periodic and chaotic oscillations [6, 7].

The problem with using multidimensional and multiparametric difference equations is that the number, types and corresponding parameters of their embedded oscillations are not known, not even approximately. Also, unlike the case of differential equations, there are no analytical methods for qualitative analysis of multidimensional discrete difference equations. Since even simple DCD mathematical models contain more than two non-linear difference equations with several parameters, finding possible types of embedded complex solutions in the form of oscillations directly from the fitting of experimental data – and subsequently subjecting these solutions to qualitative analysis – is an extremely difficult computational task.

To achieve a reasonable computational time, it is necessary to retrieve the desired type of oscillations by special methods for each particular system of difference equations before its further use for fitting of experimental data.

Therefore the inverse problem relating to the field of complex oscillatory dynamics mathematical modeling should be formulated in two steps. The first step should be to retrieve and classify all existing types of oscillations with corresponding parameters for the particular system of DCD difference equations taken from the list of initial hypotheses. If the obtained oscillations correspond qualitatively (in type and shape) to the observed experimental data, this system of equations (chosen hypotheses) should be considered as the mathematical model for further investigation in step two. Consequently, the second step should be directed to performing statistical analysis of the obtained model, using the parameters found in step one as an initial approximation for fitting of experimental data by the non-linear least square method. This will enable us to define quantitative characteristics of the adequacy of the model(s) and the confidential intervals of the model's parameters.

The multidimensional parameter space of the DCD difference equations in which the desired complex periodic and chaotic oscillations reside is composed of a multitude of isolated regions ("multitude of local optima"), and that is why formulated inverse problem is ill conditioned, requiring the development of special numerical methods.

Below we present one of the possible solutions to the first step of the inverse problem formulated above, in which we apply the heuristic search method known as the real coded genetic algorithm (RCGA) [3, 4] to retrieve and automatically classify the complex oscillations.

A genetic algorithm (GA) is a robust optimization and search technique inspired by the principle of evolution, i.e. reproduction of the population and survival of the most durable and fit individuals [5]. GAs have been adopted over the last decade to find optimal solutions in a complex irregular search space. Notable examples of their applications include the estimation of nonlinear parameters for linear and nonlinear filters, both feedforward and recurrent neural networks [17], and parameter extraction in the MOSFET model [11, 15]. RCGAs have been used to identify parameter sets in the Jiles-Atherton hysteresis model for representing nonlinear characteristics of magnetic materials [13], and to determine the equivalent circuit parameters for three-winding transformers [10]. A GA was used to produce neural network feedback controllers for chaotic systems in [16]; in [2] a GA was employed to evolve cellular automata to perform a computational task requiring globally-coordinated information processing. Based on these results, we expected that RCGAs could prove efficacious for our goal: finding as many sets of parameters corresponding to the desired oscillatory regimes as possible for a concrete system of DCD difference equations within the given computational time.

Classification of the obtained complex discrete oscillatory solutions present another computational problem. The use of classical tools such as Lyapunov exponents [14] to characterize and classify oscillations does not always give correct results, especially when the problem involves multidimensional difference equations with several parameters. The reason is that numerical procedures for calculating Lyapunov exponents are based on the calculation of derivatives that become unstable owing to the finite accuracy of computations and error propagation. We are therefore proposing to use a robust procedure for classifying oscillation types based on a direct method for checking their stability that does not involve numerically calculated derivatives.

2. BACKGROUND

According to DCD, the initial hypothesis about the mechanism of agent interactions should be given by the matrices a_{ij} and ν_{li}, and "information exchange" between the agents should be indicated [6]. The basic equations of DCD for mathematical modeling of a discrete time series yield a system of non-linear difference equations (forward problem):

$$\prod_{i=1}^{N} X_i^{\nu_{li}}(t_q) = \pi_l \tag{1}$$

$$\sum_{i=1}^{N} a_{ij} X_i(t_q) = b_j \tag{2}$$

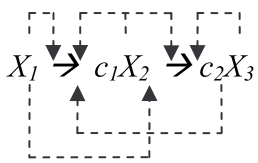
$$\pi_l = k_l \exp\left\{-\sum_{i=1}^{N} \alpha_{li} X_i(t_{q-s})\right\}, \qquad X_i(t_0) = \begin{cases} b_j, & i = j \\ 0, & i = M+1, M+2, ..., N \end{cases} \tag{3}$$

where $i = 1,2,\ldots,N$, $j = 1,2,\ldots,M$, $l = 1,2,\ldots,N-M.$,
or in the equivalent form:

$$X_{q+s} = F(X_q, \theta) \tag{4}$$

where X_i is an N component vector ($i = 1,2,...,N$) characterizing the particular state of the system during its evolution in the "discrete time" t_q ($q = 1,2,...,Q$), s is the "discrete time" delay ($s = 1,2,...$), $\theta(b_j, k_l, \alpha_{li}, \nu_{li}, a_{ij})$ is the vector of parameters, and F is the transforming function corresponding to the system of nonlinear algebraic eqns (1)-(3) that have just one positive solution $X_i > 0$ for any set of parameters θ, for any mechanism of transformation specified by ν_{li}, and for any mechanism of "information exchange" specified by the parameters α_{li}. Here the elements of the matrixes a_{ij} and ν_{li} are the real numbers, and they are regarded as the varying parameters of the model.

For purposes of illustration, here we will investigate the following mechanism of agent transformation ($N = 3,\ M = 1,\ l = 2$):



where the dotted arrows denote “information exchange”, and therefore a_{ij} and ν_{li} :

$$a_{ij} = \begin{vmatrix} 1 \\ c_1 \\ c_2 \end{vmatrix}; \quad \nu_{li} = \begin{vmatrix} -c_1 & 1 & 0 \\ -c_2 & 0 & 1 \end{vmatrix}; \tag{5}$$

In this case eqns (1)-(3) will have the following forms:

$$\frac{X_2(t_q)}{X_1^{c_1}(t_q)} = k_1 \exp\left\{-\sum_{i=1}^{3} \alpha_{li} X_i(t_{q-1})\right\} \tag{6}$$

$$\frac{X_3(t_q)}{X_1^{c_2}(t_q)} = k_2 \exp\left\{-\sum_{i=1}^{3} \alpha_{li} X_i(t_{q-1})\right\} \tag{7}$$

$$X_1(t_q) + c_1 X_2(t_q) + c_2 X_3(t_q) = b \tag{8}$$

The initial conditions according to eqn. (3) will be:

$$X_1(t_0) = b, X_2(t_0) = 0, X_3(t_0) = 0\,. \tag{9}$$

We have constrained our model here by setting $s = 1$. We also assume that:

$$\alpha_{li} = \alpha_{l'i}\,,\ l \neq l',\ \ l, l' = 1,2\,.$$

The model (6)-(8) has 8 parameters: $\theta(b, k_1, k_2, \alpha_1, \alpha_2, \alpha_3, c_1, c_2)$. The mathematical model used here corresponds to one of the initial mechanisms (eqn. (5)) of agent interactions. If the solutions obtained from the system of difference equations (in this case, eqns (6)-(8)) should fail to match the experimental data with the required accuracy, the model's complexity may be increased by introducing additional agents (constituents), by including more detailed "information exchange" (increasing the "discrete time" delay s=2,3…), etc.

We intend to perform a numerical investigation of eqns (6)-(8) in order to retrieve different types of embedded oscillations by applying a procedure of automatic search and analysis using RCGA and a fitness function specially constructed for our purpose (DCD inverse problem). A major difficulty encountered in analyzing and classifying the oscillatory solutions generated by (6)-(8) is that, as mentioned earlier, with classical methods such as calculation of the Lyapunov exponents, the attractor's fractal dimension becomes computationally unstable and fails to give the expected results for multidimensional and multiparametric difference equations. To overcome this problem, we are proposing a robust numerical procedure for classifying complex oscillatory solutions based on direct calculation of the asymptotic behavior for one of the trajectories resulting from eqns (6)-(8).

Let us investigate the asymptotic behavior of $X_1(t_q)$ ($Q \to \infty$) within its dependence on infinitesimal $\varepsilon \to 0$ introduced into the initial conditions, as follows:

$$X_1(t_0, \varepsilon_k) = b + \varepsilon_k, X_2(t_0, \varepsilon_k) = 0, X_3(t_0, \varepsilon_k) = 0 \tag{10}$$

We then calculate the "coefficients λ_k " ($k = 0,1,2,...K$), which characterize the average difference between the initially "close" trajectories $X_1(t_q)$ and $X_1(t_q, \varepsilon_k)$:

$$\lambda_k = \frac{1}{Q}\sum_{q=1}^{Q}\left|X_1(t_q) - X_1(t_q, \varepsilon_k)\right|, \tag{11}$$

$X_1(t_q)$ is the trajectory calculated for initial conditions (9), and $X_1(t_q, \varepsilon_k)$ are the trajectories calculated for the initial conditions (eqn. (10)) ($q = 1, 2, ..., Q$).

Calculation of eqns (10) and (11) starts with initial $\varepsilon_0 = \delta_1$ and is repeated K times by decreasing ε_k

$$\varepsilon_{k+1} = 0.1\varepsilon_k\,,\ k = 0,1,2,...K\,, \tag{12}$$

until the following condition is satisfied:

$$\left|\lambda_{k+1} - \lambda_k\right| < \delta_2 \tag{13}$$

δ_1, δ_2 are small adjustable parameters ($\delta_1, \delta_2 \to 0$). Then the final $\lambda^* = \lambda_K$ corresponding to $\varepsilon^* = \varepsilon_K$ are used to define the two basic types of trajectories obtained:

$$\begin{cases} \text{stable periodic oscillations} & \lambda^* \leq \varepsilon^* \\ \text{unstable periodic and chaotic oscillations} & \lambda^* > \varepsilon^* \end{cases} \tag{14}$$

It will be shown that the proposed classification leads to the correct results when the number of iterations Q is large enough and the parameters $\delta_1, \delta_2 \to 0$.

3. ESTIMATION OF PARAMETERS USING RCGA

When using an RCGA, the search parameters are encoded in chromosomes as floating point numbers, unlike the binary representation of chromosomes of a classical GA [4, 5]. Real encoding of chromosomes is recommended in cases of continuous parameters and when each of the parameters is defined within the given interval. These recommendations inspired us to apply RCGA to our inverse problem.

The parameters of the model (6)-(8) are encoded into chromosomes, each of which is a row vector of real numbers corresponding to the parameters (genes). The size of the vector is equal to the number of parameters. Each parameter varies within the intervals specified $(\theta_{\min}, \theta_{\max})$, which in our case are chosen arbitrarily under the physical constraints, whereby some of the parameters should be positive, $b, k_1, k_2, c_1, c_2 > 0$, while α_{li} may also be negative. In the example presented here, we use the following intervals: (0,10] for b, c_1, c_2, (0,200] for k_1, k_2, and [-100, 100] for $\alpha_1, \alpha_2, \alpha_3$.

We are assuming that we have no initial information about the values of the searching parameters, and therefore each chromosome in the population is initialized by applying uniform random number distribution for each parameter within its intervals.

The fitness function (f_{obj}) should reflect our goal, which is to find complex periodic and chaotic oscillations and to classify them. It should evaluate the oscillations generated by the difference equations (6)-(8) with a view to directing the automatic RCGA search to the parameters that will correspond to the desired regimes. Therefore the fitness function should be based on an algorithm capable of distinguishing between a non-oscillatory solution and damped and non-damped oscillations. We are also interested in classifying non-damped oscillations as stable periodic and unstable periodic and chaotic oscillations.

Accordingly, we propose the following algorithm for fitness function. Because we are interested only in the asymptotic behavior of the trajectories, let us designate the "period" of the trajectory $X_1(t_q)$ by the integer p, which is equal to the number of different points of the trajectory traversed in the last T iterations of eqns (6)-(8) (for example, if $Q = 1000$, $T = 500$ to exclude points of transition). For each trajectory $X_1(t_q)$ corresponding to a concrete set of parameters (chromosome), we calculate the period. If $p = 1$ (non-oscillatory solution), we set $f_{obj}= 0$. If $p > 1$, we need to characterize the oscillatory solution obtained (damped versus non-damped oscillations). In order to exclude damped oscillations from further evaluation, we examine the changes in amplitude of the trajectory's oscillations. If the amplitude decreases monotonically with time, then the oscillations may be classified as damped and $f_{obj}= -2$. Next, we evaluate the non-damped oscillations, classifying them into the two types (stable periodic ($f_{obj} = -1$) and unstable periodic including chaotic ($f_{obj} = 1$)) using the procedure described above according to rules (10)-(14).

Therefore the fitness function proposed here is encoded into one of four arbitrarily chosen integers for designation of different types of oscillatory regimes:

$$f_{obj} = \begin{cases} -2, & \text{damped oscillations} \\ -1, & \text{stable periodic oscillations} \\ 0, & \text{non-oscillatory solutions} \\ 1, & \text{unstable periodic including chaotic oscillations} \end{cases}$$

The main operators of RCGA are selection, crossover, and mutation [5]. Selection determines which chromosomes belonging to the current population will participate in the production of the next generation. The purpose of selection is to exercise a bias towards chromosomes demonstrating a better fitness. Because we are interested in finding stable periodic, unstable periodic and chaotic oscillations, the "better fitness" correspond to $f_{obj}= \{ -1, 1\}$. We used binary tournament selection adjusted to our case: chromosomes of the previous generation were divided into two groups according to their fitness function values ($f_{obj}= \{-2, -1, 0, 1\}$). The first group comprises chromosomes with $f_{obj}= \{-1, 1\}$, because such chromosomes have a higher potential for generating complex oscillations in the next generation. Therefore we want to ensure selection of at least one of these chromosomes. The second group should comprise chromosomes with $f_{obj}= \{-2, 0\}$. First and second parent chromosomes are selected randomly from the first (with $f_{obj}= \{-1, 1\}$) and the second (with ($f_{obj}= \{-2, 0\}$) group, respectively, with equal selection probability. If all the chromosomes of the previous generation belong to only one group (first or second), then both parent chromosomes are selected randomly with equal selection probability from the sum of chromosomes of the previous generation.

After selection has been completed, the crossover (or recombination) operation is performed upon the selected chromosomes in order to produce new chromosomes. Following [3], we use a simulated binary crossover (SBX) operator with crossover parameter $\eta = 5$.

As established by numerical computation, there is no significant change in the algorithm's execution of the search for a particular type of oscillations with and without mutation (the numerical experiments were performed using a random mutation operator with mutation probabilities equal to 0.1 and 0.01).

After the children populations of chromosomes have been generated and classified with the help of the fitness function, all chromosomes proceed to the next generation.

In our case, the stop criterion for the GA is the given limit of computational time or the given maximum number of RCGA generations.

If for the first fifty generations the algorithm does not converge to the oscillatory solution ($f_{obj} = \{-1, 1\}$ is not found), random mutation is applied for all chromosomes of the current population in order to enter a new area of parameter space. This means that all parameters in the population are randomly renewed by uniform random number distribution (each parameter within its given interval).

4. RESULTS

In order to check the proposed method for seeking and analyzing oscillations, we applied it to a logistic map for which all the types of oscillatory solutions were known:

$$X_{n+1} = RX_n(1 - X_n) \tag{15}$$

An RCGA search with the proposed fitness function was performed for the population of twenty chromosomes. Computing of the iterative map was begun at the initial value $X_0 = 0.5$. The allowed interval of the parameter R was fixed at (0, 5], $Q = 1000$, $T = 500$, $\delta_1, \delta_2 = 10^{-4}$. Twenty generations of the search algorithm (4 minutes of computational time (average of 40 RCGA runs) on an ordinary PC, Intel Pentium 4) were enough to identify parameter values yielding most known types of oscillatory regimes.

As Figure 1 shows, the fitness function calculated with eqns. (10)-(14) yields a good match (indication of stable and unstable oscillation regimes) with the results of oscillation classification based on Lyapunov exponents [12].

After testing the proposed method on eqn. (15), we used it to perform an automatic search for and classification of the oscillatory solutions of eqns (6)-(8). Applying "Lyapunov exponents" for evaluation of the types of oscillations resulting from this system of difference equations was unsuccessful, presumably reflecting the much greater computational complexity of the eight parameter model as compared with the single parameter logistic map (eqn. (15)).

The search for oscillations was performed for a time limit of 100 RCGA generations, population size of twenty chromosomes, $Q = 1000$, $T = 500$, and $\delta_1, \delta_2 = 10^{-4}$. 100 generations of the search took about 1.5 hours (average of 40 RCGA runs) with an algorithm written using Matlab 6.12 and run on a PC (Intel Pentium 4). Application of RCGA to the searching parameters corresponding to the different complex oscillations embedded in eqns (6)-(8) led to the identification of various complex oscillations. A partial bifurcation diagram was obtained for $-0.0654 < \alpha_1 < 2.1346$ and for the following parameter values: b = 8.2266, k_1 = 15.1561, k_2 = 159.9907, α_2 = 4.9340, α_3 = -6.3035, c_1 = 3.0015, c_2 = 6.0400 (Figure 2a).

Analysis of this bifurcation diagram was carried out by calculating the fitness function according to eqns (10)-(14) and revealed stable periodic ($f_{obj} = -1$) and unstable periodic and chaotic ($f_{obj} = 1$) oscillations (see Figure 2b). As we wanted to focus on the latter two types of oscillation, fitness function values corresponding to damped oscillations were omitted from Figure 2b.

The results of the formal classification of the oscillations obtained using eqns (10)-(14) are illustrated graphically by the corresponding trajectories (Figure 3a, b, c, d) and phase portraits (Figure 3a', b', c', d'). The periodic oscillations corresponding to the "windows" ($\alpha_1 = 1.3396, p = 12$; $\alpha_1 = 1.6346, p = 10$) revealed by the calculated fitness function (Figure 2b) are shown in Figure 3a and b. The chaotic oscillations for $\alpha_1 = 1.5496$ and $\alpha_1 = 1.8296$, f_{obj}=1 are presented in Figure 3c and d.

In principle, the RCGA method could find numerous oscillations and classify them into two basic types, each of which comprises different shapes of oscillations. These could make up a "database of oscillations" that would prove useful in the future mathematical modeling of experimentally observed data in complex dynamical systems(the second part of inverse problem). Examples of different oscillations are presented in Figure 4.

5. CONCLUSIONS

The robustness and efficiency of the proposed method for seeking and classifying the different types of complex oscillation embedded in multidimensional and multiparametric difference equations was demonstrated on a mathematical model derived from discrete chaotic physicochemical reactions dynamics. Obtained by RCGA different types of oscillations resembles experimentally observed [1, 8]. The method tested may be applied to any system of difference equations to perform an automatic search for parameters corresponding to different types of complex oscillatory solutions.

The search method presented belongs to the class of so-called "soft engineering" or "soft computing" methods, which are capable of giving a reasonable time consumption even for such complex computational problems. It provides a practical tool for qualitative analysis of complex difference equations and makes it possible to create a database of different types of oscillations for further use in fitting of real experimental data (the second part of the inverse problem discussed here).

Demonstrated ability to conduct an automatic search of required DCD mathematical models and to identify parameters of the model that correspond to the specific type of complex oscillations may be expected to facilitate the modeling, interpolation, extrapolation, optimization, and control of the dynamics of real systems by difference equations.

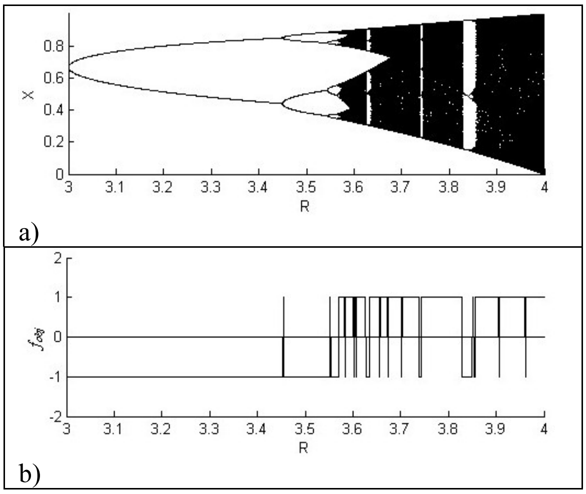


Figure 1. Bifurcation diagram and fitness function (f_{obj}) reflecting two types (stable and unstable) of oscillations generated by eqn. (15).

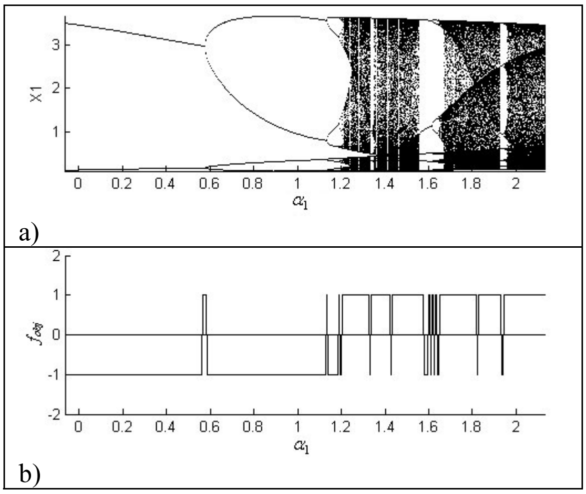


Figure 2. Bifurcation diagram and fitness function (f_{obj}) reflecting two types (stable and unstable) of oscillations generated by eqns (6)-(8).

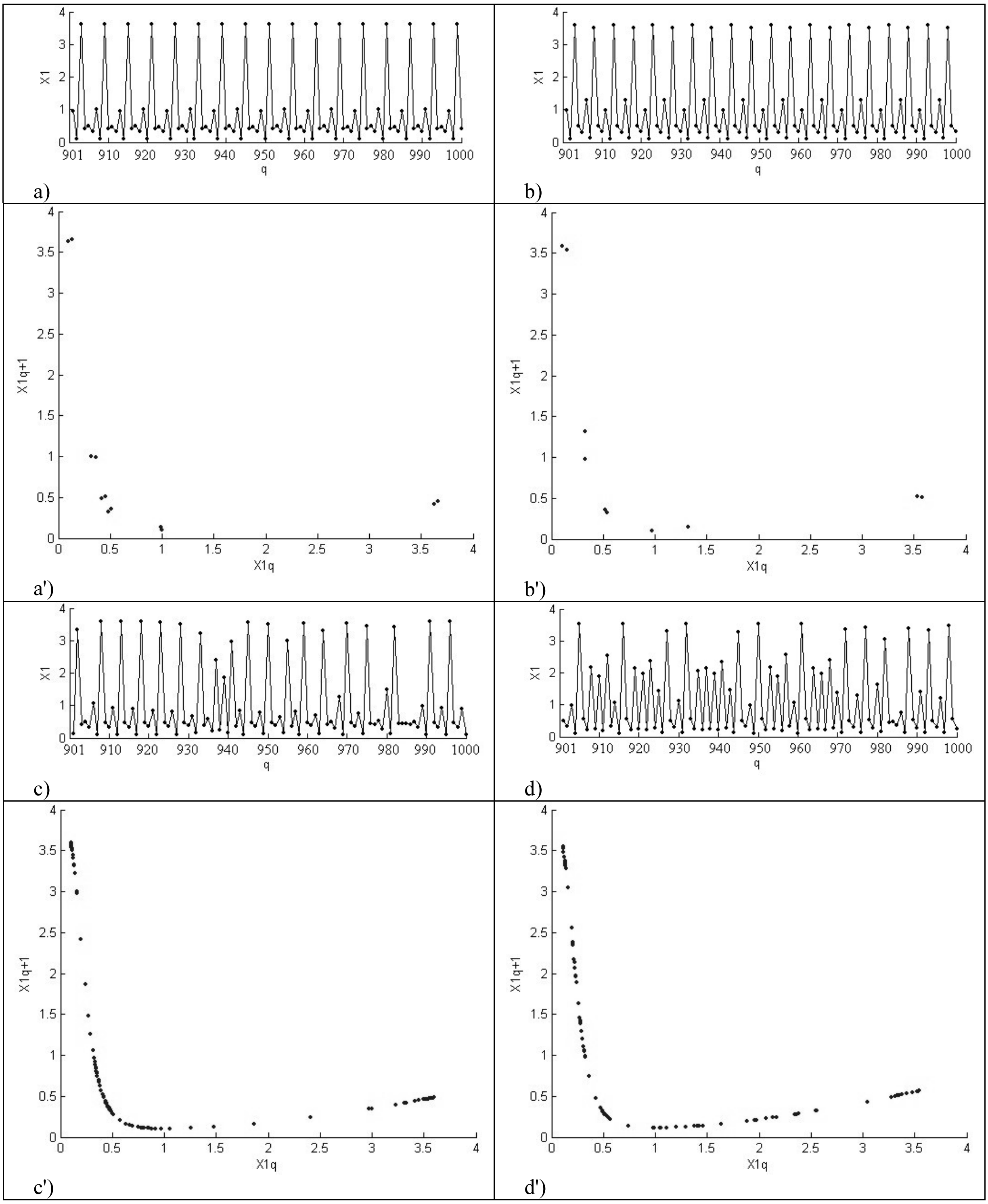


Figure 3. Time series with corresponding phase portraits.
a) $\alpha_1 = 1.3396$, $p = 12$, f_{obj}=-1; b) $\alpha_1 = 1.6346$, $p = 10$, f_{obj}=-1 ; c) $\alpha_1 = 1.5496$, f_{obj}=1; d) $\alpha_1 = 1.8296$, f_{obj}=1.

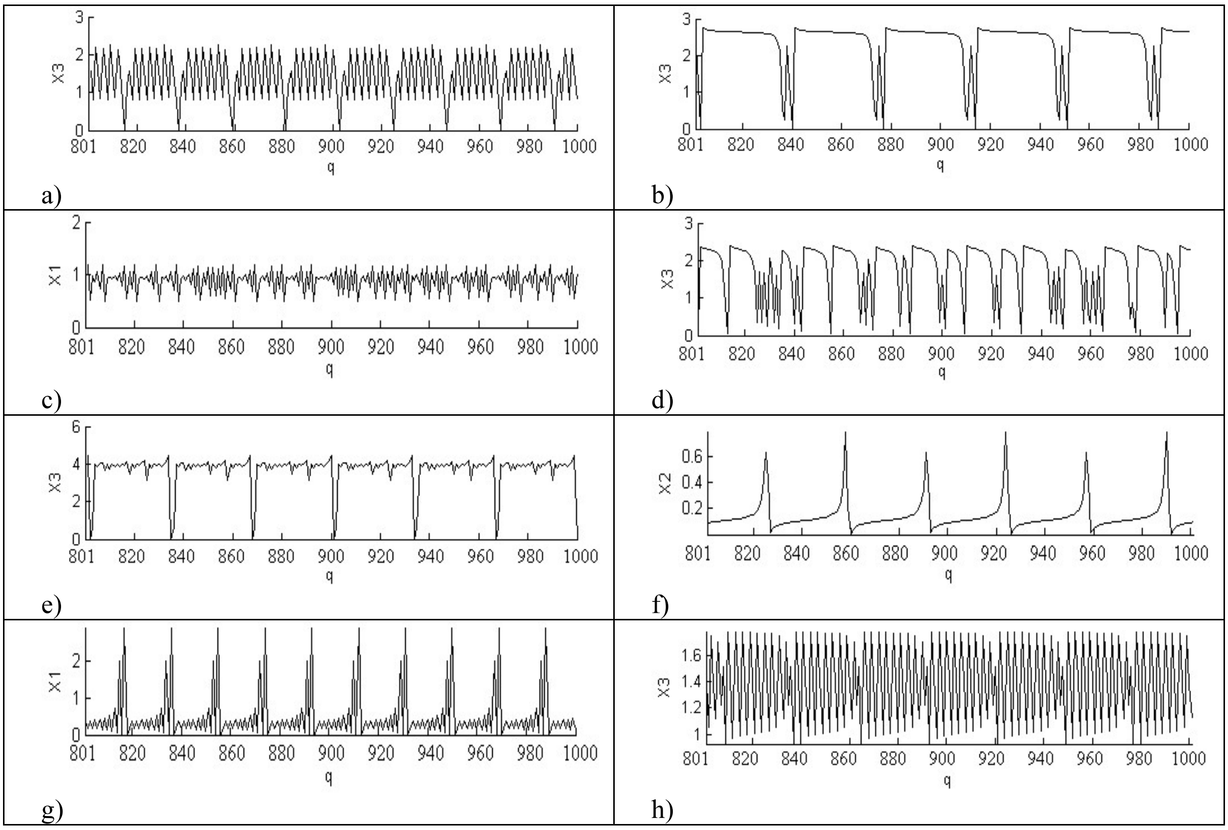


Figure 4. Examples of oscillations found by RCGA with the corresponding parameters:
a) $b = 2.3728, k_1 = 3.6221, k_2 = 4.7710, \alpha_1 = -38.9062, \alpha_2 = 10.1276, \alpha_3 = -3.3988, c_1 = 1.0959, c_2 = 1.0171$;
b) $b = 2.7532, k_1 = 6.5603, k_2 = 8.9045, \alpha_1 = -2.5234, \alpha_2 = 9.2100, \alpha_3 = -0.7457, c_1 = 1, c_2 = 1$;
c) $b = 5.7600, k_1 = 2.7502, k_2 = 8.2461, \alpha_1 = -11.3779, \alpha_2 = 0.7151, \alpha_3 = 15.7151, c_1 = 1.5591, c_2 = 5.4285$;
d) $b = 2.4000, k_1 = 6.5603, k_2 = 8.9045, \alpha_1 = -3.0000, \alpha_2 = 9.3495, \alpha_3 = -0.7457, c_1 = 1, c_2 = 1$;
e) $b = 7.7385, k_1 = 5.4585, k_2 = 1.1358, \alpha_1 = -4.4019, \alpha_2 = 2.8596, \alpha_3 = -16.0185, c_1 = 5.0695, c_2 = 1.9301$;
f) $b = 2.7500, k_1 = 6.5603, k_2 = 8.9045, \alpha_1 = -3.0000, \alpha_2 = 9.2222, \alpha_3 = -0.7457, c_1 = 1, c_2 = 1$;
g) $b = 2.8907, k_1 = 60.7765, k_2 = 0.1000, \alpha_1 = -7.5526, \alpha_2 = 2.3876, \alpha_3 = 8.0941, c_1 = 2.4027, c_2 = 0.4663$;
h) $b = 1.7892, k_1 = 2.5951, k_2 = 1.4883, \alpha_1 = -43.2614, \alpha_2 = 8.1372, \alpha_3 = -0.6643, c_1 = 1, c_2 = 1$.

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