Automatic Semiqualitative Analysis: Application to a Biometallurgical System

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Abstract. The aim of this work is the representation and analysis of semiqualitative models. Their qualitative knowledge is represented by means of qualitative operators and envelope functions. A semiqualitative model is transformed into a family of quantitative models.
In this paper the analysis of a model is proposed as a constraint satisfaction problem. Constraint satisfaction is an umbrella term for a variety of techniques of Artificial Intelligence and related disciplines. In this paper attention is focused on intervals consistency techniques. The semiqualitative analysis is automatically made by means of consistency techniques. The presented method is applied to a industrial biometallurgical system in order to show how increase the capacity of production.

1 Introduction

In engineering and science, the models made up for the study of dynamical systems are normally composed of quantitative and qualitative knowledge. This knowledge is composed by both of them. It is known as semiqualitative knowledge. Real models contain quantitative, qualitative and semiqualitative knowledge. All this knowledge must be considered when these models are studied.

The techniques developed to analyze and simulate quantitative models are well known. A great variety of techniques has been studied for the representation and the manipulation of qualitative knowledge, such as algebra of signs, interval arithmetic, fuzzy sets, and order of magnitude reasoning.

In order to analyze industrial models, it is necessary sometimes to solve conflicts on the request of accuracy and flexibility. The models of dynamical systems should provide different levels of numerical abstraction for their elements. These levels may be a purely qualitative description [8], semiqualitative [2], [6], numerical based on intervals [11], quantitative and mixed of all levels [7].

On other hand, the systems dynamics obtains the differential equations of a system from its structure. This technique could obtain different qualitative behaviors of a given structure. The analysis of these behaviors constitutes the qualitative analysis of dynamical systems. The mathematical qualitative theory of dynamical systems involved studying qualitatively the behaviour (e.g. asymptotic behaviour) of time evolving systems.

In order to automate the qualitative analysis of dynamic systems several applications have been developed. They combine techniques of numerical methods with symbolic computation, and methods proceeding from the knowledge of the science and the mathematics. These applications begin with the top-level specifications of physical model. They prepare simulation experiments, and accomplish them. Also they interpret the numerical results, and they formulate the results in qualitative terms. Among them, we can cite *PLR* [9], *bifurcation interpreter* [1], *KAM* [12], *POINCARE* [10], and *MAPS* [13]. In this paper, a method to carry out the analysis of dynamical systems automatically is shown. The semiqualitative analysis is proposed as a set of interval constraint satisfaction problems. They are solved applying consistency techniques [5].

2 Semiqualitative models

A dynamical system can be considered as the constraints

$$\Phi(\dot{x}, x, p), \qquad x(t_0) = x_0, \qquad \Phi_0(p, x_0) \tag{1}$$

being x the state variables of the system, p the parameters, $\dot{x}$ the variation of the state variables with the time, Φ_0 the constraints among parameters and initial conditions, and Φ the constraints on $\dot{x}, x$ and p. The dynamical system represented in (1) can symbolically be transformed into a set of contraints with variables, parameters and intervals. In this paper, we only study systems that can be transformed as

$$\dot{x} = \tilde{f}(x, p), \qquad x(t_0) = x_0, \qquad \Phi_0(p, x_0) \tag{2}$$

The vector field $\tilde{f}$ may be composed of quantitative and qualitative variables, constants, arithmetic operators, functions and envelope functions, expressed as it is indicated in our previous paper [4], where qualitative variables and envelope functions are transformed to interval expressions. If we take into account the stablished concepts in that paper, the dynamical system (2) is transformed in

$$\dot{x} = f(x, r, p), \qquad x(t_0) = x_0, \qquad \Phi_0(p, r, x_0) \tag{3}$$

where $r \in \mathbb{I}$ are new parameters, $p \in \mathbb{I}, x_0 \in \mathbb{I}$, and f does not contain envelope functions, being $\mathbb{I}$ the set of closed intervals of $\mathbb{R}$. These functions represent a dynamical systems family depending on p, x_0 and r. It is denoted as *semiqualitative model* and it is represented further on

$$\dot{x} = f(x, p), \qquad x(t_0) = x_0, \qquad \Phi_0(p, x_0) \tag{4}$$

where p and r have been joined in an unique parameters vector p.

3 Semiqualitative analysis

Qualitative analysis of a dynamical system intends to analyze the *phase portrait* or *phase space* of the system. The *phase space* of the dynamical system is constituted by the variables of state x, and the *extended phase space* by variables and parameters x, p. The phase portrait is formed by the projection of the trajectories of the dynamical system in the extended phase space. The phase portrait is interpreted as a correspondence between the differential equations and the vector field. In this paper semiqualitative systems that they are stable structurally are studied. In them, little perturbations keep their qualitative behaviors.

The first step of semiqualitative analysis of a dynamical system (4) is the determination of the *equilibrium regions*. They are defined by the constraints

$$Equilibrium(x,p) \equiv \{ f(x,p) = 0, \tag{5}$$

The study of solutions of (5) let us know the structure of the phase portrait. Each stable equilibrium region is an attractor region.

The *stability* of each equilibrium region is related to the real part of the eigenvalues of the Jacobian of the system. It has been demonstrated in the bibliography that in the stable fixed points the real part of the eigenvalues is negative. In order to apply the stability criteria, it is necessary to construct the following determinants. They are formed with the coefficients of the characteristic polynomial P_n of the Jacobian matrix A of the dynamical system. The Jacobian matrix of (4) is $A = D_x f(x,p)$, and P_n is defined as

$$P_n(\lambda) = det(A - \lambda I) = a_0\lambda^n + a_1\lambda^{n-1} + \ldots + a_{n-1}\lambda + a_n \tag{6}$$

In order to determine the stability conditions, the matrices are defined

$$g_i = det \begin{pmatrix} a_1 & a_3 & a_5 & \ldots & a_{2i-1} \\ a_0 & a_2 & a_4 & \ldots & a_{2i-2} \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & 0 & a_i \end{pmatrix} \text{ being } i = 1, \ldots, n \tag{7}$$

The elements a_k of g_i are the coefficients of P_n for $k > n$, and 0 for $k \leq n$. Both a_k and g_i are symbolic expressions dependent on x, p.

We can apply two stability criteria. First is the *Routh-Hourwitz criterion.* For this criterion the predicate *Stable_Pol* is defined as

$$Stable\_Pol(P_n(\lambda)) \equiv \{ g_1 > 0, \ldots, g_n > 0 \tag{8}$$

Second is the *Lineard-Chipard criterion.* It defines the predicate *Stable_Pol* as

$$Stable\_Pol(P_n(\lambda)) \equiv \begin{cases} a_1 > 0, \ldots, a_n > 0, \\ g_{n-1} > 0, g_{n-3} > 0, \ldots \end{cases} \tag{9}$$

Therefore the constraints that define the stable equilibrium regions are

$$Stable(x,p) \equiv \begin{cases} Equilibrium(x,p), \quad A = D_x f(x,p), \\ P_n = P_C(A), \quad Stable\_Pol(P_n(\lambda)) \end{cases} \tag{10}$$

where D_x stands for the Jacobian, and P_C stands for the set of constraint of characteristic polynomial. If constraints (10) are satisfied by an *equilibrium region*, it is stable. Otherwise it is not stable.

The study of the *bifurcations points* of a system intends to divide the parameters space in regions. The system has the same number and type of attractors in these regions. The frontiers of these regions are formed by bifurcation points. An attractor appears, disappears or changes of type, when we cross a determined frontier.

The most elemental classification of bifurcation points distinguishes them into statics and dynamics. The *statics bifurcation points* are the simplest. They appear in those points where the number of attractors points varies. The determinant of the Jacobian matrix is annuled in them, that is, the characteristic polynomial has a null root.

The *dynamic bifurcation points* involve *limit cycles* or *strange attractors*. We study the *Hopf bifurcation*, where an attractor point is converted into a limit cycle or vice versa. In these bifurcation points the characteristic polynomial of the Jacobian matrix has a pair of roots with real part equal to zero.

$$Sta\_Bif(x,p) \equiv \begin{cases} Equilibrium(x,p), \\ A = D_x f(x,p), \\ P_n = P_C(A), \\ P_n = \lambda\, Q_{n-1}, \\ Stable\_Pol(Q_{n-1}) \end{cases} \qquad Din\_Bif(x,p) \equiv \begin{cases} Equilibrium(x,p), \\ A = D_x f(x,p), \\ P_n = P_C(A), \quad (11) \\ P_n = (\lambda^2 + w^2)\, Q_{n-2}, \\ Stable\_Pol(Q_{n-2}) \end{cases}$$

It is interesting to notice that all the predicates defined between (5) and (11) are formuled as interval constraint satisfaction problems. They are solved by adequate consistency techniques [5].

4 A biometallurgical system

4.1 Description and determination of the model

For a long time, it has been observed natural transformations of the sulphur and iron compounds. They are originated from the dissolution of minerals. Presence of iron-oxiding bacteria in mining areas and their acid drainages has been reported repeatedly.

Thiobacillus Ferrooxidans is considered to be the most important organism for the bacterial leaching of minerals. In indirect leaching the bacteria generate ferric iron by oxidizing soluble ferrous iron. The global reaction is

$$2Fe^{2+} + 1/2O_2 + 2H^+ \Longrightarrow 2Fe^{3+} + H_2O \qquad (11)$$

This method for production of acidified ferric solutions is used because ferric iron in turn oxidizes other metals in mineral, transforming them in the soluble form, and because it avoids ecological contamination problem of industrial extraction of metals from the rocks.

If the equation of Michaelis-Mention is applied to the reaction (11), then oxidation rate V is calculated as follows

$$V = V_{max} \frac{[S]}{k_m + [S]} \tag{12}$$

where V_{max} is maximum rate that it can be reached by increasing in the substrate concentration, $[S]$ is substrate concentration, and k_m is Michaelis constant. This constant stands for the concentration which the reaction rate is half of the maximum rate. This equation has two problems: the concentration bacterian is not constant and it cannot be applied to the bacterian growth because it is exponencial. Due to the complexity of the factors that take part in the bacteria oxidation of Fe(II) in Rotating Biological Contactors (RBC), as shown in figure (1). It has not been possible to determine a general mathematical model for this process. However, it has been proved that the bioxidation reaction continues a kinetic of first order with respect to the substrate concentration. In the experimentation there are two interconnected RBC. In them it is introduced a flow Q with an ferrous iron concentration.

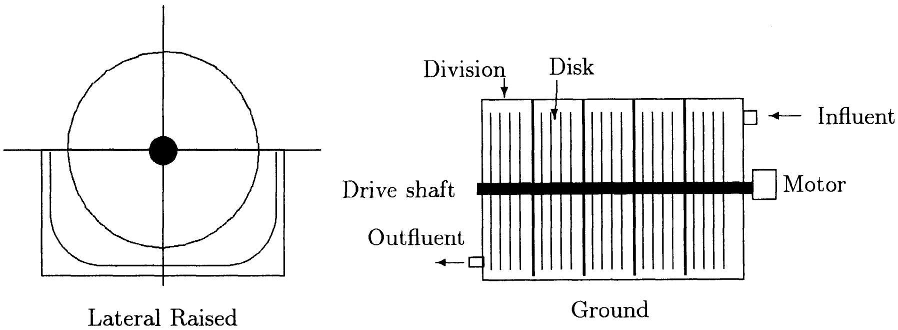

Fig. 1. A Rotating Biological Contactors (RBC)

The equations of the model of this dynamical system are

$$\begin{cases} \frac{dx_1}{dt} = \left(p_1\, p_2 - p_3\, p_4 \frac{x_1}{x_1+p_5} - p_1 x_1\right) p_6 \\ \frac{dx_2}{dt} = \left(p_1\, x_1 - p_7\, p_8\, \frac{x_2}{x_2+p_9} - p_1 x_2\right) p_{10} \end{cases} \tag{13}$$

4.2 Experimental data

According to the experimental results [3] it has been determined the quasi-equilibrium points for the system. They have been obtained studying different influent flows p_1 and values of iron concentration in such flows p_2.

According to the data supplied by the experts p_5 is similar to p_9 and their order of absolute magnitude is *moderately positive*, p_7 is *very positive*, and p_3 is *slightly greater* that p_7. Therefore, if it is associated the corresponding intervals to the previously expressed qualitative operators, it is obtained

$$p_1 = 0.61l/h, p_2 = 3.96g/l, \quad p_3 = [5.6, 5.8], p_4 = 0.74l, \qquad p_5 = [0.4, 0.5],$$
$$p_6 = 0.015, \quad p_7 = [5.3, 5.6], p_8 = 0.78l, \qquad p_9 = [0.4, 0.5], p_{10} = 0.01$$

Using these data and applying the exposed techniques, we carry out the semi-qualitative analysis of these dynamical systems.

4.3 Semiqualitative analysis

The semiqualitative analysis of this system is carried out to study how to increase the capacity of production, when systems parameters are varied. The equilibrium regions of the system are determined solving the network of contraints

$$Equilibrium(x,p) \equiv \begin{cases} (p_1\, p_2 - p_3\, p_4 \frac{x_1}{x_1+p_5} - p_1 x_1)\; p_6 = 0, \\ (p_1\, x_1 - p_7\, p_8\, \frac{x_2}{x_2+p_9} - p_1 x_2)\; p_{10} = 0, \\ 0.4 \le p_5 \le 0.5,\; 0.4 \le p_9 \le 0.5,\; 5.6 \le p_3 \le 5.8, \\ 5.3 \le p_7 \le 5.6,\; p_1 = 0.61,\; p_2 = 3.96, \\ p_4 = 0.74,\; p_6 = 0.015,\; p_8 = 0.78,\; p_{10} = 0.01 \end{cases}$$

If it is applied interval arithmetic the results obtained are too wide. Nevertheless it is applied interval consistency techniques developed in [5] and we will obtain a narrowing equilibrium region

$$Equilibrium(x,p) = \{[0.397, 0.49], \times [0.0198, 0.034]\}$$

This solution includes all experimental results obtained from different experience data.

The Jacobian matrix of this model is

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} -\frac{p_3 p_4 p_5 p_6}{(x_1+p_5)^2} - p_1 p_6 & 0 \\ p_1 p_{10} & -\frac{p_7 p_8 p_9 p_{10}}{(x_2+p_9)^2} - p_1 p_{10} \end{pmatrix}$$

The characteristic polynomial of A is

$$P_n(\lambda) = a_0\lambda^2 + a_1\lambda + a_2 = \lambda^2 + (-a_{11} - a_{22})\lambda + a_{11}a_{22} - a_{12}a_{21}$$

and according to the Lienard-Chipard criterion,

$$Stable\_Pol(P_n(\lambda)) \equiv \{\, (-a_{11} - a_{22}) > 0, a_{11}a_{22} - a_{12}a_{21} > 0$$

Substituting p_i for their values and simplifying, the constraints that define the stability are

$$Stable(x,p) \equiv \begin{cases} Equilibrium(x,p), \\ -0.00915 + \frac{0.0111[5.6,5.8]x_1}{([0.4,0.5]+x_1)^2} - \frac{0.0111[0.4,0.5]}{[0.4,0.5]+x_1} > 0 \\ -0.00915 + \frac{0.0111[5.6,5.8]x_1}{([0.4,0.5]+x_1)^2} - \frac{0.0111[5.6,5.8]}{[0.4,0.5]+x_1} - 0.0061 + \\ \frac{0.078[5.3,5.6]x_2}{([0.4,0.5]+x_2)^2} - \frac{0.078[5.3,5.6]}{[0.4,0.5]+x_2} > 0 \end{cases}$$

These constraints are satisfied with the obtained equilibrium region and therefore it is conclude that the region is stable.

The constraints that define the bifurcations are

$$Sta\_Bif(x,p) \equiv \begin{cases} Equilibrium(x,p), \\ a_1 > 0,\, a_2 = 0 \end{cases} \quad Din\_Bif(x,p) \equiv \begin{cases} Equilibrium(x,p), \\ a_1 = 0,\, a_2 > 0 \end{cases}$$

When it is applied constraint satisfaction techniques to these constraints, there are no solutions, and hence the system has no bifurcations.

5 Conclusions

This paper proposes a method to carry out automatically the semiqualitative analysis of dynamical systems by interval consistency techniques. Qualitative knowledge is represented by intervals, and they are qualitative operators and envelope functions.

It has been applied the proposed approach to systems appeared in the bibliography and the obtained results are quite similar to them. In this paper, it has been studied a real biometallurgic system. The achieved results have allowed to know how to increase the capacity of production.

In the future, we are going to apply the previous techniques to other real problems. We also want to extend the analysis process with the study of other types of attractors, dynamic bifurcations, and the incorporation of multiple scales of time, and delays.

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