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A model based fault diagnosis in a nonlinear bioreactor using an inverse problem approach

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Abstract. This paper presents a proposal of robust model based fault diagnosis in a nonlinear bioreactor, seen as a solution of an inverse optimization problem. The optimization problem is solved using the evolutionary strategy Differential Evolution (DE). The results indicate the suitability of this approach.

Keywords. fault diagnosis, robustness, inverse problem, evolutionary strategy, multiple faults

1 Introduction

A fault in a system is a non-allowed deviation of at least one property, characteristic or parameter, from its acceptable condition. The faults derive in degradation or even loss of functioning in a system [1]. For this reason, the development of fault diagnosis methods for industrial systems, which should be robust in the presence of noise or external perturbations, is a very current topic.

Among the ways of approaching this problem, the model based methods can be found [6]. Mathematical models allow to incorporate the faults affecting the system via a faults vector. The determination of the faults vector, when the input and output signals of the system are known, can be approached as the solution of an inverse optimization problem [4].

Nonlinear bioreactors are essential technology in chemical and biochemical industries. It is known that any disturbance in the nutrient concentrations that are involved in a bioreactor process can generate radical changes in its performance.

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It has been recently shown that formulating fault diagnosis by an inverse problem methodology helps obtain an appropriate balance between robustness and sensitivity [2].

In this paper, a proposal of robust model-based fault diagnosis via parameters estimation in a nonlinear bioreactor is presented, through the solution of an inverse optimization problem using the Differential Evolution algorithm.

The main contribution of this paper is the application of this method to strong nonlinear systems as bioreactors including the diagnosis of incipient and multiple faults.

This paper is organized as follows. Section 2 will present the description of the nonlinear bioreactor and the Differential Evolution algorithm. Section 3 will be devoted to results and numerical experiments. Finally, some conclusions are presented.

2 Materials and Methods

2.1 Description of the bioreactor model

In this subsection the model of the nonlinear bioreactor proposed by Contois in 1959 is described. The model depicts the velocity of the growth of microorganisms and substrate in a bioreactor using the kinetics equation of Contois [3].

Two substances are involved in the process, being ξ_1 the microorganisms concentration and ξ_2 the substrate concentration. The states vector will be $x = [x_1, x_2]^T \in \mathbb{R}^2$ where

$$\begin{aligned} x_1 &= \xi_1 \\ x_2 &= \frac{a_1 \xi_1 \xi_2}{a_2 \xi_1 + \xi_2} \end{aligned} \quad (1)$$

The process is affected by two faults f_{p1} and f_{p2} . They represent the presence of substances that alter the concentration of microorganisms. These faults are modeled by the terms

$$f_{p1} = \Psi_1 \theta_1, \quad f_{p2} = \Psi_2 \theta_2 \quad (2)$$

where $\theta_1, \theta_2 \in \mathbb{R}$ are the unknown values of the concentrations of the substances and Ψ_1, Ψ_2 are functions that determine the periodical appearance of f_{p1} and f_{p2} respectively.

The model of the system, with the faults incorporated, respond to the following system of nonlinear differential equations

$$\begin{aligned} \dot{x}_1 &= x_2 - u x_1 + \Psi_1 \theta_1 + \Psi_2 \theta_2 \\ \dot{x}_2 &= \frac{a_2 x_2 (x_2^2 - a_1 u x_1^2) + (a_1 x_1 - x_2)^2 (a_4 u - a_3 x_2)}{a_1 a_2 x_1^2} \\ x(t_0) &= x_0 \\ y &= x_1 \end{aligned} \quad (3)$$

$$y = x_1 \quad (4)$$

where the concentration of microorganisms x_1 is measured by a sensor; $a_1, a_2, a_3, a_4 \in \mathbb{R}$ are model parameters and $u \in \mathbb{R}$ is the input function of the system that represents the dilution rate, which acts as the control variable.

Since functions Ψ_1 and Ψ_2 have a known behavior, the estimation of faults f_{p1} and f_{p2} is focused in the estimation of values of θ_1 and θ_2 . The diagnosis of the faults is carried out by solving the optimization problem:

$$\begin{aligned} \min F(\hat{\theta}_1, \hat{\theta}_2) &= \sum_{t=1}^I \left[y_t(x_1, x_2, \theta_1, \theta_2, u) - \hat{y}_t(\hat{x}_1, \hat{x}_2, u, \hat{\theta}_1, \hat{\theta}_2) \right]^2 \\ \text{s.t. } &\theta_{1 \min} \leq \hat{\theta}_1 \leq \theta_{1 \max} \\ &\theta_{2 \min} \leq \hat{\theta}_2 \leq \theta_{2 \max} \end{aligned} \quad (5)$$

where $\hat{y}_t(\hat{x}_1, \hat{x}_2, \hat{\theta}_1, \hat{\theta}_2, u)$ is the estimated output of the system at each time t that is obtained by solving the system (5) and $y_t(x_1, x_2, \theta_1, \theta_2, u)$ is the real output of the system measured at the same time t by a sensor. I is the number of measurements of the input ($u(t)$) and output ($y(t)$) vectors.

Figure 1 shows a diagram of the fault estimation as the solution of an inverse optimization problem.

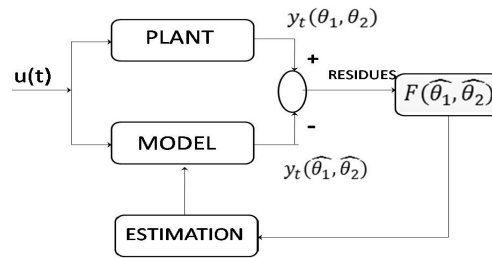


Figure 1: Diagram of the fault estimation process.

2.1.1 Simulation of the bioreactor

The model parameters, the dilution rate u and the values of the faults used in the simulations are the proposed in [7]. The bioreactor parameters will be $a_1 = a_2 = a_3 = 1, a_4 = 0.1$. The function describing the dilution rate is

$$u(t) = \begin{cases} 0.08 & \text{if } 0 \text{ h} \leq t < 10 \text{ h} \\ 0.02 & \text{if } 10 \text{ h} \leq t < 20 \text{ h} \\ 0.08 & \text{if } t \geq 20 \text{ h} \end{cases} \quad (6)$$

Three experiments were done. The first in the presence of fault f_{p1} ($\theta_1 = 0.01, \theta_2 = 0$), the second with the presence of fault f_{p2} ($\theta_1 = 0, \theta_2 = 0.015$) and the last one in the presence of both faults simultaneously ($\theta_1 = 0.01, \theta_2 = 0.015$). The functions

$$\Psi_1(t) = \begin{cases} 0 & \text{if } 0 \text{ h} \leq t < 20 \text{ h} \\ 1 & \text{if } t \geq 20 \text{ h} \end{cases} \quad \Psi_2(t) = \begin{cases} 0 & \text{if } 0 \text{ h} \leq t < 30 \text{ h} \\ 1 & \text{if } t \geq 30 \text{ h} \end{cases} \quad (7)$$

will describe the appearance of these faults in time.

The output of the system is affected by Gaussian noises that represent 2,5,8,10,12 or 15% of the variable x_1 . All the implementations were made in MATLAB R2012a.

Figure 2 shows the output of the bioreactor simulated without the presence of faults (a) and with both faults present at the same time, respectively (b). In both cases there are not noise.

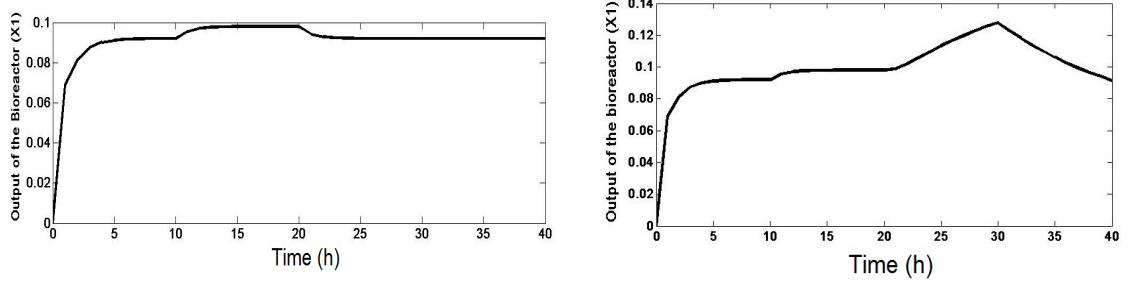


Figure 2: Output of the bioreactor without fault and with both faults.

2.2 Differential Evolution (DE) Algorithm

Differential Evolution, DE, was proposed in 1995 for optimization problems [5]. Some of the most important advantages of DE are: simple structure, simple computational implementation, speed and robustness [5]. DE is based on three operators: *Mutation*, *Crossover* and *Selection* [5]. These operators are based on vector operations, which are their main difference from Genetic Algorithms [4]. At each iteration $Iter$ the algorithm generates a new population of Z feasible solutions $X_{Iter}^1, X_{Iter}^2 \dots X_{Iter}^Z$ with the application of its three operators on the current population. This mechanism can be summarized with the notation:

$$DE/X_{Iter-1}^\delta/\gamma/\lambda \tag{8}$$

where γ indicates the number of pairs of solutions from the current population to be used for perturbing the present solution X_{Iter-1}^δ ; λ represents a distribution function to be used during *Crossover*. This paper applied the scheme $DE/X^{best}/2/bin$, where bin is a notation for a binomial distribution function and *Mutation* is described by:

$$X_{Iter}^z = X^{best} + C_{scal} (X_{Iter-1}^{\alpha 1} - X_{Iter-1}^{\alpha 3} + X_{Iter-1}^{\alpha 2} - X_{Iter-1}^{\alpha 4}) \tag{9}$$

where $X^{best}, X_{Iter-1}^{\alpha 1}, X_{Iter-1}^{\alpha 2}, X_{Iter-1}^{\alpha 3}, X_{Iter-1}^{\alpha 4} \in \mathbf{R}^n$ are solutions from the current population and C_{scal} is an algorithm's parameter, called *Scaling factor*. *Crossover* and *Selection* operators can be described as:

- *Crossover*

$$\hat{x}_{(Iter)n}^z = \begin{cases} \hat{x}_{(Iter)n}^z & \text{if } q_{rand} \leq C_{cross} \\ \hat{x}_{(Iter)n}^\delta & \text{otherwise} \end{cases} \tag{10}$$

where $\hat{x}_{(Iter)n}^z$ are components from vector $\hat{\mathbf{X}}_{Iter}^z$; $0 \leq C_{cross} \leq 1$ is another algorithm's parameter: *crossover factor*; and q_{rand} is a random number that is generated by means of the distribution represented by λ .

- *Selection*

Vector \mathbf{X}_{Iter}^z to be part of a new population, is selected using the following rule:

$$\mathbf{X}_{Iter}^z = \begin{cases} \hat{\mathbf{X}}_{Iter}^z & \text{if } F(\hat{\mathbf{X}}_{Iter}^z) \leq F(\mathbf{X}_{Iter-1}^\delta) \\ \mathbf{X}_{Iter-1}^\delta & \text{otherwise} \end{cases} \quad (11)$$

A general description of the algorithm for DE optimization algorithm is shown in Figure 3.

Require: $Z, MaxIter, C_{scal}, C_{cross}$
Ensure: \mathbf{X}^{best}

- 1: Generate an initial population of Z solutions
- 2: Select best solution \mathbf{X}^{best}
- 3: **for** $Iter \leftarrow 1, MaxIter$ **do**
- 4: Apply *Mutation*
- 5: Apply *Crossover*
- 6: Apply *Selection*
- 7: Update \mathbf{X}^{best}
- 8: Verify stopping criteria
- 9: **end for**
- 10: Solution: \mathbf{X}^{best}

Figure 3: Algorithm for the Differential Evolution method (DE).

3 Results and Discussion

Three experiments were conducted considering 6 different levels of noise. The first experiment was realized considering the presence of the fault θ_1 only. The second experiment was done considering the presence of the fault θ_2 . The third experiment considers that the two faults appear simultaneously. Two stopping criteria were used at every case: reaching a maximum number of iterations or a relative error in the estimations of θ_1 and θ_2 .

Applying a commonly used statistical procedure in this kind of experiments, 25 runs of the DE algorithm were made for each case of faults. The results obtained were filtered using quartiles. In other words, the solutions were put in ascending order and the data belonging to the first and fourth quartile were eliminated. This process was carried out with the objective of removing possible outliers that could appear. Then, it was calculated the average of: the estimated faults $\hat{\theta}_1, \hat{\theta}_2$, the value of the objective function $F(\hat{\theta}_1, \hat{\theta}_2)$, the amount of evaluations of the objective function \overline{Eval} and the amount of iterations of the algorithm \overline{Iter} .

3.1 Experiments

In order to conduct the experiments, the following values were used in the implementation of the DE algorithm: $Z = 20$, $C_{esc} = 0.6$ and $C_{cross} = 0.9$. A maximum number

of 200 iterations and a relative error of 5% in the estimations of θ_1 and θ_2 were used as stopping criteria.

3.2 Numerical results

Tables 1, 2 and 3 show the experimental results.

Table 1: Experiment 1 $\theta_1 = 0.01$, $\theta_2 = 0$

% of noise	$\overline{\hat{\theta}_1}$ (0.01)	$\overline{\hat{\theta}_2}$ (0)	$\overline{F(\hat{\theta}_1, \hat{\theta}_2)}$	\overline{Eval}	\overline{Iter}
2 %	0,009856165	0,000368202	0,000220776	284	12
5 %	0,010058863	-0,000725862	0,000966661	1176	56
8%	0,010700311	0,00221580	0,003335268	3746	185
10 %	0,00837417	-0,004486296	0,00407326	4040	200
12 %	0,009605867	-0,000973501	0,005209922	2880	142
15 %	0,013009417	0,00848987	0,011615478	4040	200

Table 2: Experiment 2 $\theta_1 = 0$, $\theta_2 = 0.015$

% of noise	$\overline{\hat{\theta}_1}$ (0)	$\overline{\hat{\theta}_2}$ (0.015)	$\overline{F(\hat{\theta}_1, \hat{\theta}_2)}$	\overline{Eval}	\overline{Iter}
2 %	-0,000304156	0,014993854	0,000189863	323	14
5 %	0,000366912	0,015213365	0,000748552	278	11
8%	0,000056384	0,014947312	0,001735661	307	13
10 %	-0,00020687	0,014135388	0,003102743	2032	99
12 %	-0,000573714	0,013333792	0,003379113	3456	170
15 %	0,000405394	0,016392316	0,006562496	2915	143

Table 3: Experiment 3 $\theta_1 = 0.01$, $\theta_2 = 0.015$

% of noise	$\overline{\hat{\theta}_1}$ (0.01)	$\overline{\hat{\theta}_2}$ (0.015)	$\overline{F(\hat{\theta}_1, \hat{\theta}_2)}$	\overline{Eval}	\overline{Iter}
2 %	0,00997806	0,014945478	0,000109994	301	13
5 %	0,009557908	0,015213365	0,001155813	1464	71
8%	0,009725932	0,015441528	0,002277264	2015	98
10 %	0,010045468	0,016505602	0,004581219	3747	185
12 %	0,010029644	0,016102557	0,005010786	2884	142
15 %	0,008469452	0,014899756	0,010186071	3464	171

After the analysis of the experiments is possible to conclude the following:

- The estimation error increases as the noise grows. However, in all cases the estimation error is small. This demonstrate the robustness of the proposal.
- The estimation of multiple faults is a current investigation topic. Table 3 shows the excellent results obtained when the two faults f_{p1} and f_{p2} occur simultaneously.

- The bioreactor is a strongly non-linear system. However, the results of the experiments show the feasibility of the proposal because the mean value of the objective function $F(\hat{\theta}_1, \hat{\theta}_2)$ is close to zero even when the noise is high.
- The main drawback of this algorithm could be the computational cost. However, the dynamic of a bioreactor is in general very slow, then, the possible computational cost is not a difficulty in this case.

4 Conclusions

In this paper, an approach to robust fault diagnosis in a chemical nonlinear bioreactor was developed using the solution of an inverse optimization problem. To solve the optimization problem the Differential Evolution algorithm was used. The obtained results demonstrate the feasibility of the proposal. As future works, the behavior of other evolutive algorithms will be analyzed.

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