ROBUST PARAMETERS IDENTIFICATION OF THE OXYGEN KINETICS USING THE MAXIMUM ENTROPY PRINCIPLE

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Abstract. *The purpose of this paper is to identify the parameters that characterize the curve of oxygen absorption rate of a person during controlled physical activity (with intensity classified as heavy or severe). The values of the oxygen absorption rate were measured experimentally through the process of pulmonary ventilation in the Ergospirometry and kineanthropometry Laboratory - LErC of Federal University of Rio de Janeiro. The oxygen absorption rate after the onset of exercise is described in terms of a mono or multiple-component exponential function. Each exponential is identified as a distinct physiological stage and represents the body's response to increased energy metabolism. The characterization of the curve for each patient requires the identification of the number of phases developed during the exercise, and identification of the instants when the change of phase occurs. The study of oxygen kinetics has become a powerful important tool in clinical medicine. It provides important information about the severity and progression or regression of specific pathologies. The dynamic response of pulmonary gas exchange reflects the integrated response of the ventilator, cardiovascular, and neuromuscular systems. The parameter identification made in this paper takes into account the uncertainties of the process. One computer code is developed to solve a robust optimization problem. The Maximum Entropy Principle is used to construct the probability density function of the random variables of the oxygen kinetics. And the Monte Carlo simulations are employed to compute the mean and variance at each point of the robust optimization. The results are compared to the ones of the deterministic optimization, and compared to the parameter identification made by the nonlinear least squares method.*

Keywords: *identification, optimization, stochastic modeling, maximum entropy principle*

1. INTRODUCTION

The physical exercise in human beings involves rather sudden transitions from one metabolic rate to another. The requirement of increasing energy metabolism during physical activity is directly related with the Oxygen Uptake Kinetics (v_o), which involves the study of the physiological mechanisms responsible for the dynamic v_o response to physical activity (Jones and Poole, 2005).

The oxygen kinetics as a parameter of physiological function became a standard laboratory measurement. The measurement of v_o represents the values of the oxygen absorption rate of a person during controlled physical activity.

To determine the parameters values that best characterizes the curve of v_o is necessary to solve an optimization problem. Since it takes into account the uncertainties of the process it is named robust optimization (RO). As the robust optimization may have two objective functions (e.g., minimize the mean and the variance), its formulation is in the form of a multi-objective optimization problem. To deal with multi-objective optimization the weighted sum have been employed.

In this paper, the uncertainties on the parameters of the oxygen kinetics are taken into account by modeling them as random variables. To do so, the parametric approach is used and the probability density functions are derived using the Maximum Entropy Principle (Shannon, 1948; Jaynes, 1957a,b). Monte Carlo simulations are employed to compute the mean and variance at each point of the robust optimization.

This paper is organized as follows. The oxygen kinetics is presented in Section 2 and the probabilistic model is presented in Section 3. The robust optimization problem is defined in Section 4 and the optimization algorithm is explained in Section 5. Finally, the numerical results are presented in Section 6 and the concluding remarks are given in Section 7.

2. OXYGEN KINETICS

The measurement of v_o kinetics has become an important tool in the evaluation of the extent of dysfunction and in some instances the mechanism behind that dysfunction in many major chronic disease conditions. The capability for v_o kinetics determination to provide insights into physiologic function and pathophysiologic dysfunction accounts in large part for the recent explosion in publications in this area.

The study of v_o is important because oxidative metabolism is the principal means by which the human organism generates energy to do work in the most short-lived activities. Factors such as the highest attainable v_o and the rate at which v_o rises in the transition to an activity with a higher energetic requirement to reach the requisite steady-state level, will all influence an individual's tolerance to physical activity.

The metabolic and gas exchange responses to controlled exercise is related to a number of identifiable exercise intensity domains (namely: moderate, heavy, severe and extreme), and to the fitness level of the individual. The systematic physical training results in physiological and biochemical body adaptations, leading to improved performance of specific tasks. The nature and magnitude of these changes are dependent on the type of activity performed, intensity, and genetic load.

The time course of the v_o response after the onset of exercise has been described in terms of a mono or multiple-component exponential function (Jones and Poole, 2005). Each exponential represents body's response to the exercise and is characterized by the development of a physiological phase.

In this paper, a simple model of v_o is considered in order to focus on the robust optimization strategy used. The curve of modeled by a mono-exponential Eq. (1), and characterizes the increase in v_o at exercise onset caused by elevated pulmonary blood flow.

$$v_o(t) = vo_{bl} + a_c(1 - e^{(-t/\tau_c)}) \tag{1}$$

where:
vo_{bl} = rate of oxygen consumption at rest (base line) $[ml/(Kg.min)]$
a_c = asymptotic constant $[ml/(Kg.min)]$;
τ_c = time constant $[1/s]$;

The vector, x, of parameters that characterizes the curve of v_o is:

$$x = (vo_{bl},\ a_c,\ \tau_c)^T \tag{2}$$

To determine the x value that best characterizes the curve of v_o is necessary to solve an optimization problem. The objective is to determine the vector $x^\star$ which minimizes the distance, d, of sum of squares residuals between the curve and the measurements values of v_o. In a deterministic problem, the objective function would be defined as:

$$x^\star = arg\ min \left\{ \sum_{i=t_1}^{t_f} \left[v_{o\ i} - v_o(x,i)\right]^2 \right\} \tag{3}$$

$$d(x) = \sum_{i=t_1}^{t_f} \left[v_{o\ i} - v_o(x,i)\right]^2 \tag{4}$$

where $t_1, \cdots, t_f$ represent the instants of the v_o measurements values.

3. PROBABILISTIC MODEL

Several methods have been developed for on-line breath-by-breath calculation of v_o. From the middle of the 1960s to 1980s, computer algorithms for measuring v_o at the mouth over a single respiratory cycles were developed (Jones and Poole, 2005). A breath-by-breath system measures airflow or volume continuously and simultaneously determines instantaneous gas concentrations. However, this process generates unique problems related to the often high variability between breaths that leads sometimes to a noise signal. Besides this, the v_o parameters represent one try of measurer the integrated response of the human body systems to the exercise. Thus, there are uncertainties in the values of the v_o parameters.

Assuming that the three parameters are independent random variables, a probabilistic approach has been employed to model the uncertainties on VO_{bl}, A_c and T_c (the capital letter is used for the random variables). The Maximum Entropy Principle has been used to construct the probability density function of each random variable. The known information used to do this is:

1. The parameters values are always positive: $VO_{bl} > 0$, $A_c > 0$ and $T_c > 0$.
2. The mean values are known: $E[VO_{bl}] = \underline{vo}_{bl}$, $E[A_c] = \underline{a}_c$ and $E[T_c] = \underline{\tau}_c$.
3. The conditions: $E[ln(VO_{bl})] < +\infty$, $E[ln(A_c)] < +\infty$ and $E[ln(T_c)] < +\infty$. This information is used because 0, and values near to it, should be repulsive values for VO_{bl}, A_c and T_c.

Taking into account the above available information and using the Maximum Entropy Principle yield the following probability density functions of VO_{bl}, A_c and T_c:

$$p_{VO_{bl}}(vo_{bl}) = \mathbb{1}_{]0,+\infty]}(vo_{bl}) \frac{1}{\underline{vo}_{bl}} \left(\frac{1}{\delta^2_{VO_{bl}}}\right)^{\frac{1}{\delta^2_{VO_{bl}}}} \frac{1}{\Gamma(1/\delta^2_{VO_{bl}})} \left(\frac{vo_{bl}}{\underline{vo}_{bl}}\right)^{\frac{1}{\delta^2_{VO_{bl}}}-1} \exp\left(-\frac{vo_{bl}}{\delta^2_{VO_{bl}}\underline{vo}_{bl}}\right) \tag{5}$$

$$p_{A_c}(a_c) = \mathbb{1}_{]0,+\infty]}(a_c) \frac{1}{\underline{a}_c} \left(\frac{1}{\delta^2_{A_c}}\right)^{\frac{1}{\delta^2_{A_c}}} \frac{1}{\Gamma(1/\delta^2_{A_c})} \left(\frac{a_c}{\underline{a}_c}\right)^{\frac{1}{\delta^2_{A_c}}-1} \exp\left(-\frac{a_c}{\delta^2_{A_c}\underline{a}_c}\right) \tag{6}$$

and

$$p_{T_c}(\tau_c) = \mathbb{1}_{]0,+\infty]}(\tau_c) \frac{1}{\underline{\tau}_c} \left(\frac{1}{\delta^2_{T_c}}\right)^{\frac{1}{\delta^2_{T_c}}} \frac{1}{\Gamma(1/\delta^2_{T_c})} \left(\frac{\tau_c}{\underline{\tau}_c}\right)^{\frac{1}{\delta^2_{T_c}}-1} \exp\left(-\frac{\tau_c}{\delta^2_{T_c}\underline{\tau}_c}\right) \tag{7}$$

Thus, VO_{bl}, A_c and T_c are Gamma random variables. The $\delta_{VO_{bl}}$ δ_{A_c} and δ_{T_c} are the coefficients variation ($\delta_i = \sigma_i/\underline{i}$, where σ_i) is the standard deviation. The $\Gamma(y) = \int_0^{+\infty} t^{y-1}e^{-1}\, dt$ is the Gamma function defined for $y > 0$.

The random vector of parameters, X, is:

$$X = (V0_{bl},\ A_c,\ T_c)^T \tag{8}$$

4. ROBUST PARAMETERS IDENTIFICATION

In the deterministic optimization problem, the objective is minimize the distance, d, of sum of squares residuals between the curve and the measurements values of v_o. The objective function is defined by Eq. (3). In the associated stochastic problem, the oxygen kinetics will be a random variable V_o and, consequently, the distance is also a random variable D. This distance is defined as:

$$D(\underline{x}) = \sum_{i=t_1}^{t_f} [v_{o\,i} - V_o(\underline{x}, i)]^2 \tag{9}$$

where $\underline{x}$ is the mean value of the parameter vector $\underline{x} = (\underline{VO}_{BL},\ \underline{A_c},\ \underline{\tau_c})^T$.

$$J^\star = arg \min_{\underline{x}\,\in\,\mathcal{C}_{adm}} J(\underline{x}) \tag{10}$$

where J encompasses statistical characteristics of the random variable D, and the feasible set is defined as:

$$\mathcal{C}_{adm} = \{\underline{x} = (\underline{vo}_{bl},\ \underline{a}_c,\ \underline{\tau}_c); vo_{bl\ min} \le \underline{vo}_{bl} \le vo_{bl\ max},\ a_{c\ min} \le \underline{a}_c \le a_{c\ max},\ \tau_{c\ min} \le \underline{\tau}_c \le \tau_{c\ max}\} \tag{11}$$

The proposed form of objective function in the RO is minimize simultaneously the mean and variance of D (respectively $E[D(\underline{x})]$ and $var[D(\underline{x})]$). Thus, the robust optimization is characterized by a multi-objective problem (R H Lopez and de Cursi, 2009).

Multi-objective optimization often involves comparing about different objectives functions, with units and/or significantly different orders of magnitude,making comparisons difficult. Thus, it is usually necessary to transform the objective functions such that they all have similar orders of magnitude. Although there are many approaches, the most robust approach is known as normalization (Arora, 2004). With the normalization method, the components of objective function vector could be combined (weighted sum method) to form a scalar objective function.

The normalization method transforms the objective functions, regardless of their original range. It is given as follows (Marler and Arora, 2004; Maler and Arora, 2005):

$$E[D(\underline{x})]^{\text{norm}} = \frac{E[D(\underline{x})] - E^\star}{E^{max} - E^\star} \tag{12}$$

and

$$E[var(\underline{x})]^{\text{norm}} = \frac{var[D(\underline{x})] - var^\star}{var^{max} - var^\star} \quad (13)$$

where $E^\star$ and $var^\star$ are the Utopia points. E^{max} and var^{max} are defined as:

$$E^{max} = \max_{1 \le j \le 2} E[D(\underline{x}_j^\star)] \quad (14)$$

and

$$var^{max} = \max_{1 \le j \le 2} var[D(\underline{x}_j^\star)] \quad (15)$$

where $\underline{x}_j^\star$ is the vector that minimizes the jth objective functions (mean and variance in our case). Applying the weighted sum method, the components of objective function vector could be combined, and the objective function becomes:

$$J(\underline{x}) = \alpha E[D(\underline{x})]^{\text{norm}} + (1-\alpha) E[var(\underline{x})]^{\text{norm}} \quad (16)$$

The $\alpha \in [0, 1]$ is the weighting factor. The function J is minimized for different values of α between 0 and 1 in order to construct the Pareto frontier obtaining trade offs between the two objectives of the problem.

5. THE ROBUST OPTIMIZATION ALGORITHM

The simplest approach to minimize the objective function defined by Eq. (16) is a random search, where a new point is randomly generated and examined. It is kept if its performance is better than the previous iteration, if not it is rejected and the old point is kept. The stopping criterion of the global optimization is the maximum number of function evaluations n_max defined a priori by the user.

The Monte Carlo simulations are employed to compute the mean and variance of D Eq. (9) at each point of the robust optimization. In the simulations, the feasible set of the vector $\underline{x} = (\underline{VO}_{BL}, \underline{A_c}, \underline{\tau_c})^T$ could be determined from the parameters vector, x, obtained by the deterministic optimization problem solution.

The deterministic optimization requires a nonlinear least squares method. Thus the identification of the parameter vector, x, is made method of Levenberg-Marquardt (K Madsen and Tingleff, 2004; Lima and Sampaio, 2010).

The feasible set of the vector $\underline{x}$ used in the simulations is:

- $0.9\ vo_{bl} \ \le\ \underline{vo}_{bl} \ \le\ 1.1\ vo_{bl}$
- $0.9\ a_c \ \le\ \underline{a}_c \ \le\ 1.1\ a_c$
- $0.9\ \tau_c \ \le\ \underline{\tau}_c \ \le\ 1.1\ \tau_c$

The values of coefficients variation used are: $\delta_{VO_{bl}} = 0.015$, $\delta_{A_c} = 0.015$ and $\delta_{T_c} = 0.015$.

6. RESULTS

With the objective of studying the oxygen kinetics, one group of professors and students of UFRJ (Universidade Federal do Rio de Janeiro) made laboratory measurements of the v_o rate in a group of twenty healthy women. For each patient, the values of v_o were measured by the pulmonary ventilation during the performance of a controlled exercise with intensity classified as heavy or severe. In this section of the paper is showed the results obtained for two of the patients of the group of twenty healthy women.

6.1 Deterministic optimization results

The results of the deterministic optimization problem are shown in Fig. 1 and Fig. 2. The identification of the parameter vector, x, and minimization of the objective function Eq. (4) were made by the nonlinear least squares method of Levenberg-Marquardt.

6.2 Convergence of the stochastic solution

Monte Carlo simulations are employed to compute the mean and variance at each point of the robust optimization. The typical convergence curves for the estimator of the mean and variance of D are shown in Fig. 3 and Fig. 4. In all the numerical experiments, the sample size used is 2000.

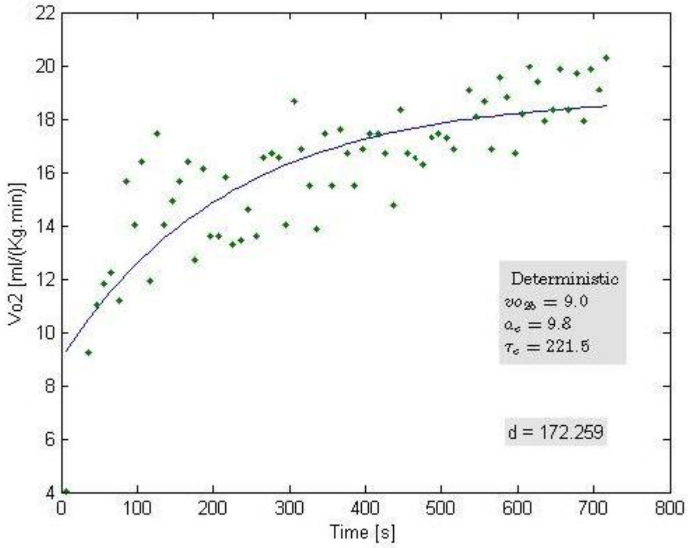

Figure 1. Vector, x, of parameters identified by the deterministic optimization for the first patient.

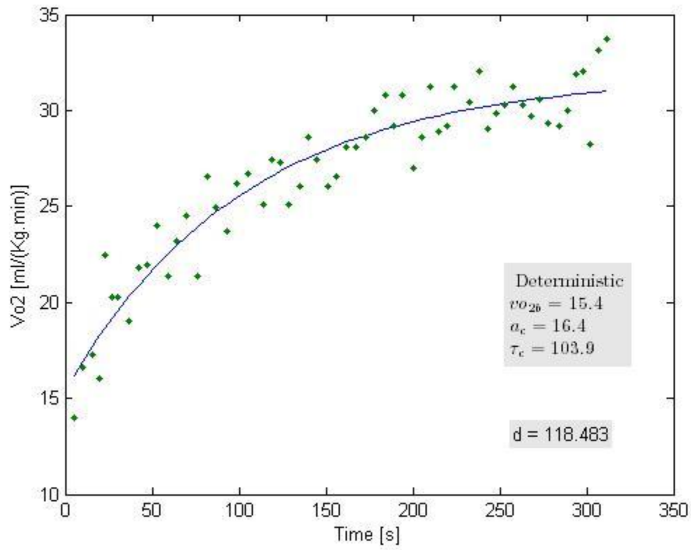

Figure 2. Vector, x, of parameters identified by the deterministic optimization for the second patient.

6.3 Pareto front

The results in the objective space, formed by the normalized values of $E[D(\underline{x})]$ and $var[D(\underline{x})]$, are shown in Fig. 5 and Fig. 6. The trade-off between the mean and the variance can clearly be observed. For each α value considered, different values of optimal mean and optimal variance are obtained.

The results of the robust optimization using different values of α are shown in Tab. 1 and Tab. 2. It can be seen that when the value of α changes, different optimal results are obtained. The higher the α is, the better the mean value of the response is and the worse the variance of response is.

Table 1. Results of the multi-objective optimization.
First patient.

α	$E[D(\underline{x})]$	$var[D(\underline{x})]$
0.00	175.46	47.97
0.20	174.97	48.17
0.50	174.51	48.97
0.80	174.47	49.24
1.00	174.40	49.96

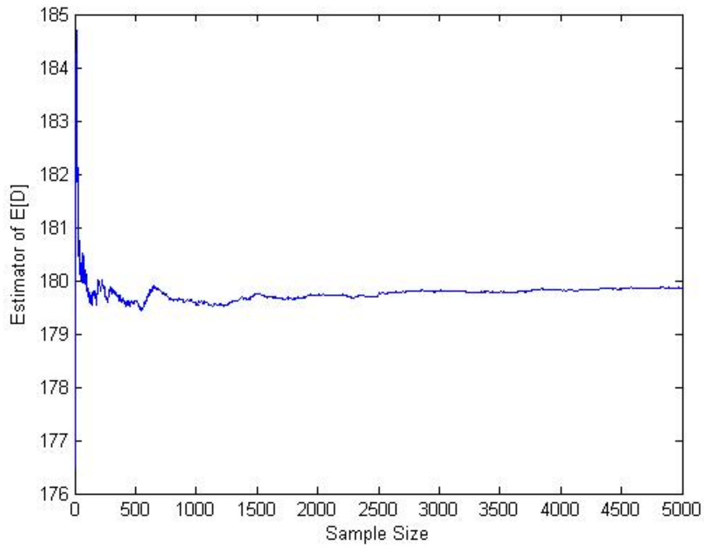

Figure 3. Convergence of the mean.

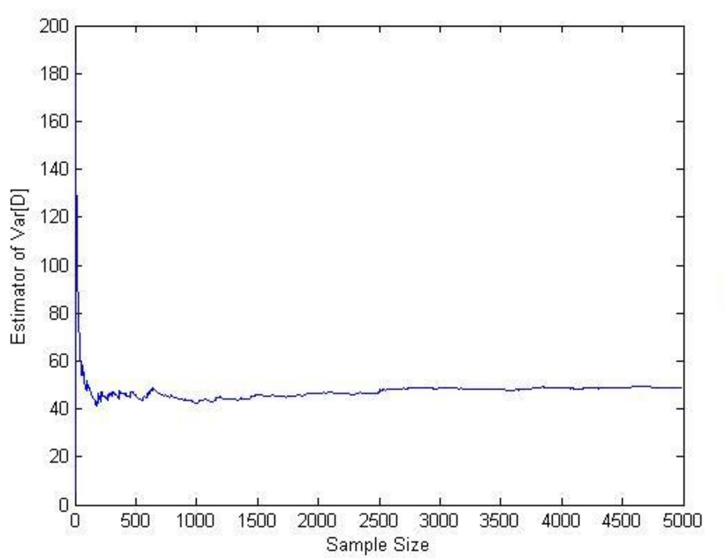

Figure 4. Convergence of the variance.

Table 2. Results of the multi-objective optimization.
Second patient.

α	$E[D(\underline{x})]$	$var[D(\underline{x})]$
0.00	124.18	42.64
0.20	123.70	43.24
0.50	123.64	43.63
0.80	123.56	44.99
1.00	123.50	47.58

7. CONCLUDING REMARKS

The purpose of this paper was identifying the parameters that characterizes the curve of oxygen absorption rate of a person during controlled physical activity. To take into account the uncertainties of the parameters, the parametric approach was used and the probability density functions were derived using the Maximum Entropy Principle.

One robust optimization problem was defined and one computer code was developed in MATLAB to solve this opti-

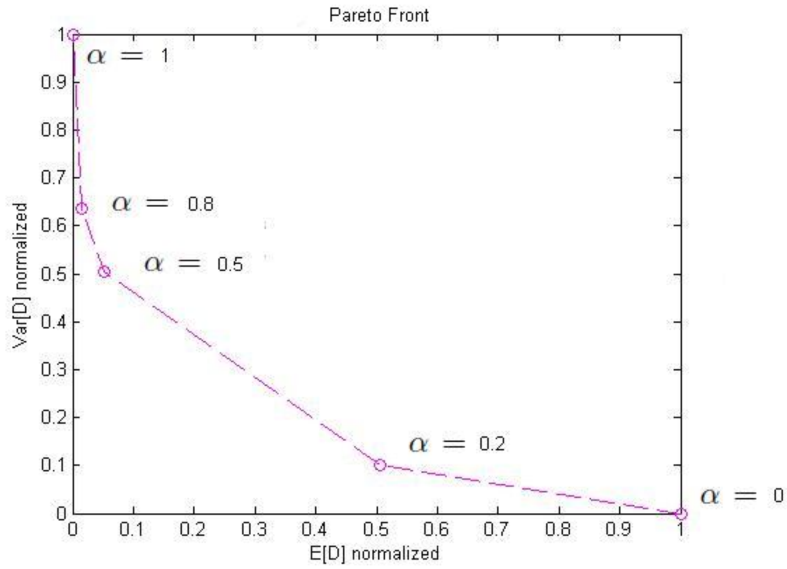

Figure 5. Pareto Front for the first patient.

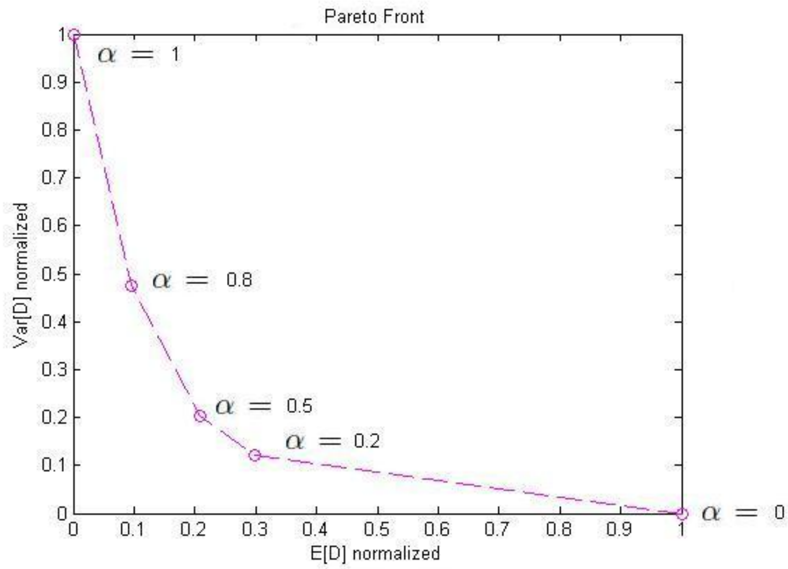

Figure 6. Pareto Front for the second patient.

mization problem. Monte Carlo simulations are employed to compute the mean and variance at each point of the robust optimization. The results showed that when the uncertainties are considered, the robust optimum design is different from the deterministic optimization optimum.

8. ACKNOWLEDGEMENTS

This work was supported by the Brazilian Agencies CNPQ, CAPES and FAPERJ.

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