

Estimating Real Process Derivatives in on-Line Optimization

A Review

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Abstract: The solution of the Integrated System Optimization and Parameter Estimation (ISOPE) problem necessitates the calculus of real process output derivatives with respect to the inputs. This information is needed in order to satisfy first and second order optimality conditions. Several methods exist and have been developed for calculating these derivatives. In this paper a review of most of the existing methods is presented, in which the Finite Difference Approximation, Dual Control Optimization, Broydon's method, Dynamic Model Identification, with both linear and nonlinear models, together with a neural networks scheme are presented and applied, under simulation, to a cascade Continuous Stirred Tank Reactor (CSTR) system. The results are then discussed and compared to identify the advantages and disadvantages of using each method.

1 INTRODUCTION

The requirement for processes to operate at their optimum operating condition is becoming increasingly prevalent. One model-based algorithm that has been developed and which can achieve optimum process operation in spite of model-reality mismatch is the Integrated System Optimization and Parameter Estimation (ISOPE) algorithm (Roberts, 1979). One requirement of the ISOPE algorithm, in order to satisfy the necessary optimality conditions, is the need for estimates of real process derivatives. These derivatives are estimated on-line at each iteration of the algorithm. The finite difference method originally used by Roberts (1979) to estimate these derivatives has proven not to be efficient in the case of large, slow and noisy processes (Mansour and Ellis, 2003). Alternative methods have therefore been developed. The dynamic model identification technique, which is based on the identification of a dynamic model, was incorporated within the ISOPE algorithm by Zhang and Roberts (1990). Although this technique proved to be fast enough as it performs the identification during transient, it encountered some difficulties such as: the huge amount of data needed and the poor, inaccurate, model it produces at the beginning of the identification. After that, an algorithm with dual control effect was proposed (Brdys and Tatjewski, 1992). In this algorithm the current

control signal is generated to satisfy the main control goal and at the same time provide sufficient information for future identification action. The main advantage of this algorithm is that it does not need excessive set-point changes to estimate the process derivatives. However, this method encountered the same type of problems as the previous ones. Broydon's approximation method based on the well-known Broydon's family of formulas which are mainly oriented to the approximation of derivatives was also implemented (Fletcher, 1980). Lately, a nonlinear version of the dynamic model identification was applied and implemented (Mansour and Ellis, 2003). In this paper, a review of all these techniques together with a method based on artificial neural networks is presented. In addition, a comparison is made using simulations carried out on a cascade CSTR system to show the advantages and disadvantages of each method.

2 THE OPTIMIZATION PROBLEM AND THE ISOPE ALGORITHM

We The ISOPE algorithm (or modified two steps) was proposed by Roberts (Roberts, 1979) to solve the general optimization problem of finding the

optimum operating point of a system while it is moving from one operating point to another. It uses an adaptive steady-state model of the process, in which the parameters are updated periodically by comparing model outputs with those of the real process.

The general form of the algorithm is given as follows (Mansour and Ellis, 2008):

Apply the current input \tilde{v}_k to the real process and wait for the system to settle down to obtain steady-state measurement \tilde{y}_k^* . Then use the existing mathematical model to determine the model parameters $\tilde{\alpha}_k$ to minimize the comparison index given by:

$$\begin{aligned} \underset{\tilde{\alpha}}{\text{Min}} \quad & G(\tilde{u}, \tilde{\alpha}) \\ \tilde{y} = & H(\tilde{v}) \\ g(\tilde{u}, \tilde{\alpha}) \leq & 0 \end{aligned} \quad (1)$$

where

$$G(\tilde{u}, \tilde{\alpha}) = \sum_{i=1}^r \tilde{w}_i (\tilde{y}_i^* - h_i(\tilde{u}, \tilde{\alpha}))^2 \quad (2)$$

and \tilde{w} is a weighting vector.

Solve the modified model-based optimization problem given by:

$$\begin{aligned} \underset{\tilde{u}}{\text{Min}} \quad & (Q(\tilde{u}, H(\tilde{u}, \tilde{\alpha})) - \lambda \tilde{u}) \\ \tilde{y} = & H(\tilde{v}) \\ g(\tilde{u}, \tilde{\alpha}) \leq & 0 \end{aligned} \quad (3)$$

In order to obtain the new candidate \tilde{u}_{k+1} .

Where

$$\lambda = \left[\left[\frac{\partial \tilde{y}}{\partial \tilde{v}} \right]^T - \left[\frac{\partial \tilde{y}^*}{\partial \tilde{v}} \right]^T \right] \left[\frac{\partial \tilde{y}}{\partial \tilde{\alpha}} \right]^{-1} \left[\frac{\partial Q}{\partial \tilde{\alpha}} \right] \quad (4)$$

λ is called a modifier and is obtained following consideration that the necessary optimality conditions, of the system optimization problem, have to be satisfied (Roberts, 1979; Ellis et al., 1988; Roberts and Williams, 1981).

However, the new control \tilde{u}_{k+1} is not directly applied to the system for stability reasons. Instead, the following relaxation scheme is used:

$$\tilde{v}_{k+1} = \tilde{v}_k + K(\tilde{u}_{k+1} - \tilde{v}_k) \quad (5)$$

where K is a relaxation gain matrix and is a tuning parameter.

These steps are repeated until convergence is reached. Convergence occurs when no further improvement is observed. In other words, when the new control is no longer a better candidate than the previous one and the objective function has reached its minimum within the possible bounds determined by the equality and inequality constraints

However, and from the previous cited relations, it can be seen that the requirement of the ISOPE algorithm to measure real process output derivatives with respect to the set-points $[\partial \tilde{y}^* / \partial \tilde{v}]$ to

compute the modifier λ imposes a practical limitation to the technique. These process derivatives are calculated online, usually by applying small perturbations on the set-points and measure the resulting changes on the outputs. This process is repeated at each iteration of the algorithm.

Various techniques exist and have been developed and applied for the purpose of estimating these derivatives. The Finite differences technique was originally suggested with the modified two step method (Roberts, 1979). Dynamic Model Identification (DMI) using a linear model was then applied by Zhang and Roberts (1990). An algorithm for dual control effect was also suggested and implemented (Brdys and Tatjewski, 1992). Also, a method based on the well known Broydon Formula was proposed and tested (Fletcher, 1980). Lately, DMI with a nonlinear model was proposed and implemented on a two CSTR system (Mansour and Ellis, 2003). In this work, a method based on Artificial Neural Networks (ANN) to estimate the real process derivatives and predict future control actions is presented. In this method, a static neural network model of the real system is created, trained and adapted to the behavior of the system. This model, imitates the behavior of the real system within its limits. The aim is to use this steady-state model to estimate the real system output derivatives with respect to the set-points in order to compute the parameter λ . All the above techniques are implemented and tested under simulation on a two CSTR system.

3 SIMULATIONS AND RESULTS

In order to assess and compare the performances of the techniques mentioned above, a set of simulations were carried out on a two Continuous Stirred Tank Reactors (CSTR) connected in cascade (Garcia and Morari, 1981). An exothermic autocatalytic reaction takes place in the reactors with interaction taking

place in both directions due to a recycle of 50% of the product stream into the first reactor.

The reaction is:



The manipulated variables which are the set-points of the temperature controllers in both reactors are:

$v = (T_1, T_2)^T$. The product concentrations associated with the second tank are outputs: $y = (Ca_2, Cb_2)^T$.

The objective function for all the simulations using this system was chosen to be linear of the measured variable and reflects the desire of maximizing the amount of component B in tank 2. Thus the form of the objective function is as follow:

$$H(y, v) = -Cb_2 \quad (7)$$

The simulations were carried out using a MATLAB®/ Simulink platform. The starting point which is the initial steady-state condition was chosen to be: $T_1(0)=307 K$ and $T_2(0)=302 K$ which yields the following steady-state outputs: $Ca_2=0.0141[kmol/m^3]$ and $Cb_2=0.0586[kmol/m^3]$.

In the simulations, the identification of the dynamic model within the DMI method (with linear or non-linear model) was carried out during transient, once found the updated model was used in the model-based optimization routine to produce the new process set-points. The identifier parameters were chosen as given in Table 1.

Table 1: Tuning the identifier parameters.

	Linear Model	Non-linear Model
Length of data window	$N_d = 120$	$N_d = 60$
Model orders	$n_a = 2, n_b = 5, n_c = 1, d = 1$	$d = 1$
Identifier sampling time	$T_s = 60s$	$T_s = 60s$
Relaxation gain	$K = 0.03I$	$K = 0.1I$

For the neural network scheme, a feedforward back-propagation neural network composed of eight input neurons, five hidden layers and two output neurons was used in the simulation. In a feedforward network, the first layer has weights coming from the input. Each subsequent layer has a weight coming from the previous layer. The last layer is the network output.

It has to be mentioned that the choice of the number of layers and their neurons depend totally on the experimenter. The main factor to be taken into account is the algorithm behaviour towards the

different values tested. In practice, the algorithm can be tested with different combinations of layers in simulations based on robust models of the system. The optimum (best) choice is then applied on the real system.

The final converged results of the simulations for the various techniques are shown in Table 2 and figures 1 to 6.

Table 2 gives the final objective function value and the number of set-point changes taken to converge to the optimum point, obtained using all the techniques presented in this paper. While the figures show the trajectories taken by the outputs and manipulated variables.

We notice that all the methods converge to the correct process optimum point given by $T_1=312 K$ and $T_2=310.2K$ with the optimum objective function value of -0.0725. From Figures 1 to 6, it is seen how the changes in the set-points affect the measured outputs and how they derive their values from the initial steady-state condition given by $Ca_2(0)=0.041361 [kmol/m^3]$, $Cb_2(0)=0.058638 [kmol/m^3]$ to the final desired solution ($Ca_2=0.0275 [kmol/m^3]$, $Cb_2=0.0725 [kmol/m^3]$).

Table 2: ISOPE algorithm with the different estimation techniques.

	Objective function value	Number of set-point changes
FDAM	-0.0725	22
Broydon's method	-0.0725	12
Dual control method	-0.0725	14
DMI with linear model	-0.0725	12
DMI with non-linear model	-0.0725	10
Neural network method	-0.0725	7

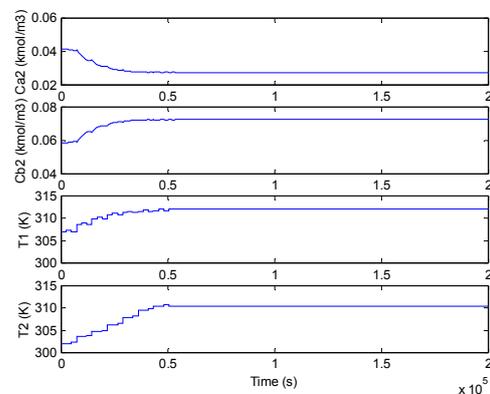


Figure 1: FDAM method.

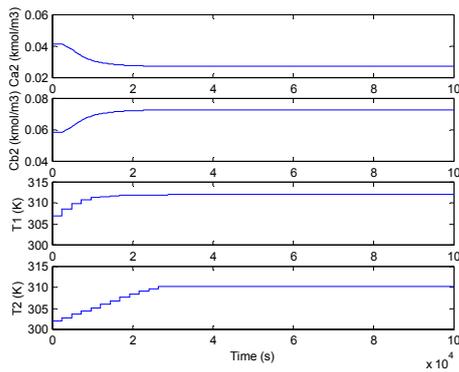


Figure 2: Broydon's method.

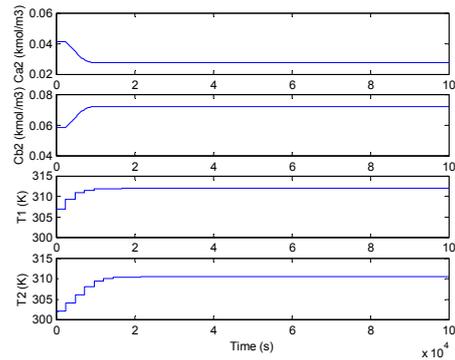


Figure 6: The Neural network method.

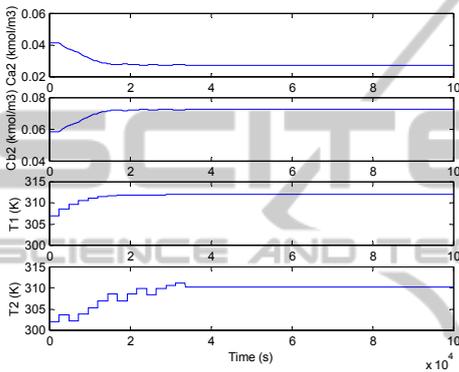


Figure 3: Dual control method.

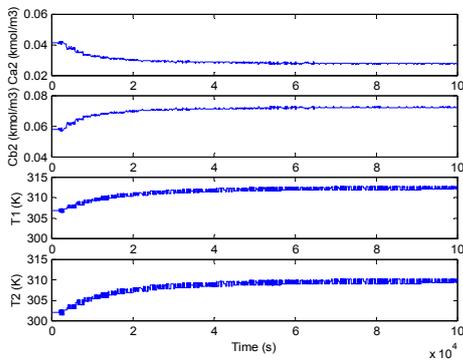


Figure 4: DMI with a linear model.

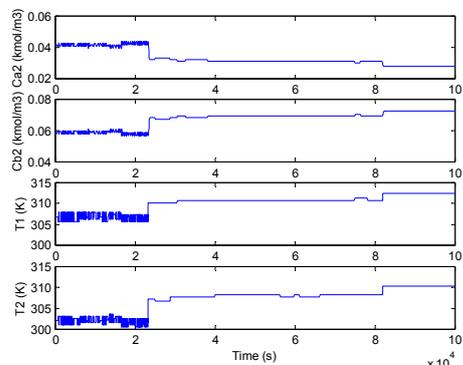


Figure 5: DMI with a nonlinear model.

4 DISCUSSION AND CONCLUSIONS

Techniques for estimating real process derivatives to be used within the ISOPE algorithm have been reviewed, and applied on a cascade process consisting of two Continuous Stirred Tank Reactors. All methods, due to the satisfaction of optimality conditions, do achieve the real process optimum provided they can be implemented in a stable manner after a suitable choice of relaxation gains.

In the case of high order, slow and noisy processes, the FDAM, is not, as is well documented, a good choice. Each time a process derivative is requested, a set-point perturbation needs to be applied and a measurement time needs to be given to allow the process to settle before the derivatives are measured. Additional difficulties are observed when noise is present on the output measurement. This set-point perturbation, and the subsequent measurement time, is where the majority of time is spent in the algorithm so this is a major consideration in assessing the algorithm. As can be seen from the simulation results on the CSTR's system (Table 2), the FDAM, approaches twice the number of set-point changes of the various after methods and would seem not to be the perfect choice of algorithm.

The dual control method takes 14 set-point changes (Table 2) to achieve the optimum in the CSTR's simulation. This is still more than the after methods but the ability of the algorithm to estimate the derivatives without any excess in the set-point changes makes it a good choice. It has to be mentioned that the ISOPE using the dynamic model identification with a nonlinear model gives better results than that using a linear one. This is demonstrated by the number of set-point changes

taken to reach the optimum point which is fewer in the first method. In this paper and using the CSTR example, the most suitable method is the neural network scheme as only 07 set-point changes are needed in order to converge to the right optimum point. However, the huge amount of data needed for training the network is its major drawback.

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