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A MIXED GA/NLP APPROACH FOR REAL-TIME OPTIMIZATION SYSTEMS BASED ON GREY-BOX NEURAL MODELS

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Abstract

This paper deals with the solution of the Real Time Optimization problem (RTO) based on grey-box neural type models. For the design of the RTO we used a dynamical grey-box type model, based on first principles and neural networks, called grey-box neural models (GNM). Previous results for this type of models showed that the solution to the GNM/RTO problem by Nonlinear Programming (NLP) fail in finding the global optimum, due to that the use of neural networks can introduce multimodal objective functions. To cope with this problem, the use of Genetics Algorithms (GA) was also investigated, finding better results than NLP approach but giving solutions near to the global optimum. Based on these previous results, we develop and test a mixed GA/NLP scheme to reach the global optimum of the RTO problem.

Keywords: Real Time Optimization, Neural Networks

1. Introduction

The online optimization of chemical plants has enjoyed considerable industrial interest because of it capacity to achieve competitive advantages in the marketplace. Numerous successful applications of the real-time optimization in industrial practice have been reported (Nath and Alzein ,2000). The economic performance of an RTO system is measured by the expected profit achieved, which is strongly influenced by the quality of the model used. The RTO systems reduce the plant/model mismatch by updating the model using actual and historical plant data sets (Yip and Marlin, 2002). Because the RTO execution is time consuming, simple phenomenological steady state models are currently used. In practical situations, however, it is difficult to reach the steady state among each RTO execution period, leaving the plant in a permanent state of slow dynamic changes. Under this condition the model is not entirely consistent and an inefficient update process could reduce the economic performance of the plant. The key to solve this problem is the use of phenomenological dynamical plant models, that have the disadvantages of being difficult to obtain and difficult to update in real time.

An alternative way of solving this difficulty is the use of dynamical models, based on combinations of first principles and neural networks (NN), called grey-box neural models (GNM). A GNM normally consists of a phenomenological part (heat and/or mass balances differential equations) and an empirical part (a neural network in this work). Due to the inherent flexibility of NN, models based on this structure are well suited to represent complex functions such as those encountered in chemical reaction processes. This work proposes incorporate in the RTO system a dynamical GNM of the plant based on phenomenological principles and neural networks. The model update is equivalent to the network training. But, the main reason for the use of this approach is the fact that a steady state equivalent model may be easily derived from the dynamical GNM and used efficiently in the optimization step.

2. Grey-box neural models (GNM)

Grey-box Neural Models combine a phenomenological model of the system with neural networks, which estimate the uncertain parameters of the process. This technique enables the synthesis of simpler mathematical models than purely phenomenological ones, with more robust generalization properties than purely NN models. These two properties make the GNM especially attractive in tasks associated with Process Identification, Process Control and Optimization, (Cubillos and Lima, 1998;, Xion and Jutan , 2002). The GNM technique consists on formulating a process model, formed by equations derived from phenomenological principles - such as mass, energy and momentum balances - and neural networks, dedicated to estimate those parameters difficult to model or uncertain. This form of representation is an attempt to add prior knowledge to black-box neural models, in order to reduce its complexity and improve their adaptive and predictive properties (Psichogios and Ungar, 1992). Thompson and Kramer (1994) classified these grey-box models into two main types: NN bringing intermediate values (parameters or variables) to be used by the phenomenological model (*series grey-box models*) or NN in parallel with the dynamic model compensating the plant/model mismatch (*parallel grey-box models*). Figure 1 shows the series scheme for a Grey-box model as used in this work.

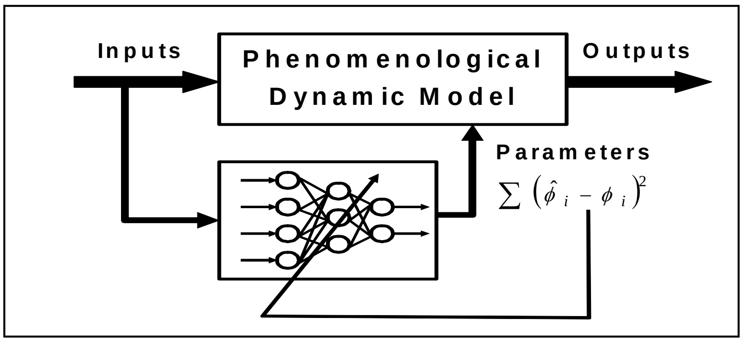

Figure 1 : The GNM approach

3. Process descriptions

In this work we applied the proposed approach to the simulated CSTR reactor from the Otto-Williams benchmark plant modified by Forbes and Marlin (1996) that may be described by elementary kinetics. The reaction sequences are:

$$\mathbf{A + B \rightarrow C} \qquad (1)$$
$$\mathbf{B + C \rightarrow P + E}$$
$$\mathbf{C + P \rightarrow G}$$

Instantaneous profits can be expressed as a function of the feed and product flow rates as (Forbest et al.,1994)

$$P = 1143.38*X(P)*Fr + 25.92\ X(E)*Fr - 76.23*Fa - 114.34*Fb \qquad (2)$$

The ideal CSTR had no reactor temperature dynamic, and the manipulated variables to optimize where the reactor temperature Tr and flow rate of B component (Fb). Fa and M were set to [2 kg/s, 10220 kg]. X(i) are the actual mass fraction of (i) component.

GNM synthesis

The GNM was synthesized considering the non stationary mass balance for each species. Feedforward neural networks were added to estimate the hypothetical reaction rates with unknown kinetics. Target reaction rates were calculated directly from discretized mass balances over a sample time To. For example, E component balance may be used to estimate the reaction rate R2 given by:

$$R2_k = ((Fa+Fb)*X(E)/2*M)_k + (X(E)_k - X(E)_{k-1})/To \qquad (3)$$

With R2 the reaction rate for the second reaction (mass based), M the mass holdup in the reactor, and X(E) the mass fraction of E component. In order to obtain adequate data to the estimation of the reaction rates, random input sequences in Fb and Tr were introduced, using a sample time of 1000 sec. Operation conditions and outlet concentrations were register to train the neural networks. The model update that consists of the NN adaptation was carried out using a second order recursive algorithm. The best NN structures were found by a systematic training procedure, considering outlet concentrations of A and B components and the reactor temperature as the inputs to the networks. Finally, networks with one hidden layer with four nodes and sigmoidal activation functions were selected.

Based on the updated dynamic GNM it was possible to derive an equivalent steady state model able to be used for optimization purposes.

Considering the model approximation, in the steady state the model equations are:

$$
\begin{aligned}
&Fa - (Fa+Fb)*X(A) - R1*M &&= 0 \qquad (4)\\
&Fb - (Fa+Fb)*X(B) - (R1 + R2)*M &&= 0\\
&- (Fa+Fb)*X(C) + (2R1 - 2R2 - R3)*M &&= 0\\
&- (Fa+Fb)*X(P) + (R2-0.5R3)*M &&= 0\\
&- (Fa+Fb)*X(E) + 2*R2*M &&= 0\\
&- (Fa+Fb)*X(G) + 1.5*R3*M &&= 0
\end{aligned}
$$

Figure 2 shows the prediction of the outlet concentration for E product using the dynamic GNM model, showing that the GNM scheme is able to adequately track the process dynamic.

4. RTO results

The GNM approach was tested in the RTO scheme considering similar operation conditions as used by Forbes and Marlin (1996), with feed flow rate and reactor temperature as the optimization variables. The optimization problem is to maximize the profit, as indicated in Equation 2, constrained by the corresponding dynamical GNM model. Previous results for this problem (Cubillos & Lima, 2003-a) showed that the solution to the GNM/RTO problem by NLP fail in finding the global optimum, due to that the use of neural networks can introduce multimodal objective functions as is showed in Figure.(3) To cope with this problem, the use of Genetics Algorithms (GA) was also investigated (Cubillos & Lima, 2003-b) giving better results than NLP approach but finding solutions near to the global optimum. Based on these previous results, we develop and test a mixed GA/NLP scheme to reach the global optimum of the RTO problem.

For this problem, in each RTO execution, the method starts with a short GA (50 data pair and 10 generations) to find a zone containing the global optimum. Subsequently, a NLP algorithm, starting with a random point inside this zone, is used to find the global optimum. The results with the GA/NLP method have shown an excellent behavior, better than the methods before mentioned, both in the stability of the algorithm as in the optimum quality reached. Test carried out in a dynamical environment achieved a 99% of effectiveness to find the GNM model optimum starting from several non optimum operational conditions. Obviously, the computational complexity of this approach is bigger than the one required by each method separately, about of 50% of increment of float point operations in each iteration.

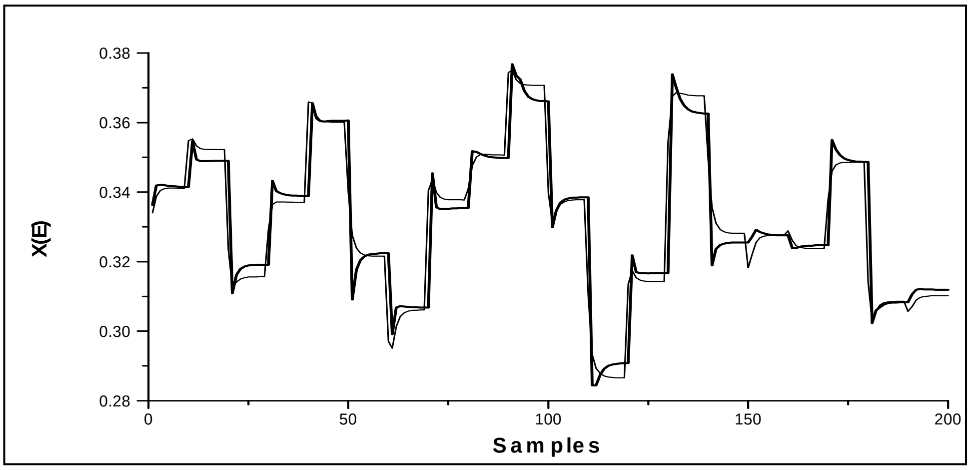

Figure 2: Actual (cont) and prediction (dash) E concentration by GNM/M2 model

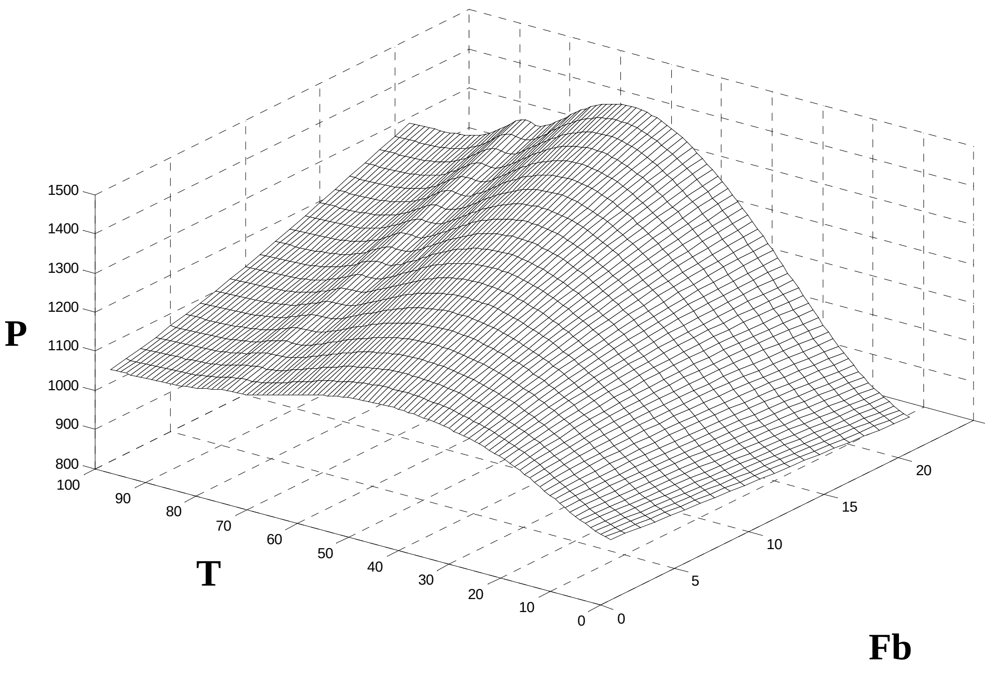

Figure 3 : Profit Surface of GNM model

5. Conclusions

The obtained results demonstrate the feasibility of the use of the GNM models in the RTO technology in a dynamic fashion. We considered that this approach introduce improvements in the RTO technology, allowing extension to highly non linear plants, feasibility of on-line adaptation using dynamical information and the integration among MPC – RTO systems by using current plants models. Considering that the GNM modeling can introduce multimodal functions, a mixed optimization strategy based on Genetics algorithm and NLP was appropriate to solve this problem.

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