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HIERARCHICAL CONTROL AND OPTIMISATION OF THE TENNESSEE EASTMAN PROCESS

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Abstract: Based on integrated system optimisation and parameter estimation a method is described for on-line steady state optimisation which compensates for model-plant mismatch and solves a non-linear optimisation problem by iterating on a linear - quadratic representation. The method requires real process derivatives which are estimated using a dynamic identification technique. The utility of the method is demonstrated using a simulation of the Tennessee Eastman benchmark chemical process *Copyright © 2002 IFAC*

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1. INTRODUCTION

An important application of numerical optimisation is the determination and maintenance of optimal steady-state operation of industrial processes, achieved through selection of regulatory controller set-point values. The implementation scheme is of a two-layer hierarchical structure as shown in Figure 1. Note that the steady-state values of the outputs are determined by the controller set-points assuming, of course, that the regulatory controllers maintain stability. The set points are calculated by solving an optimisation problem, usually based on the optimisation of a performance criterion (index) subject to a steady-state mathematical model of the industrial process. Typical performance criteria are chosen in terms of maximising profit, minimising costs, achieving a desired quality of product and minimising energy usage. Inevitably, the steady-state model will be an approximation of the real industrial process, the approximation being both in structure and parameters. We call this the 'model-reality difference problem'.

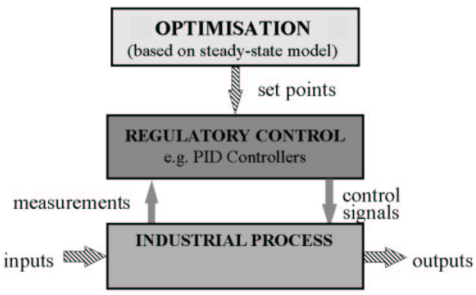

Fig. 1. Two-layer hierarchical structure

The technique known as "Integrated System Optimisation and Parameter Estimation", ISOPE, has been specifically designed to deal with the model-reality difference problem. The ISOPE technique has been developed for an extensive range of steady-state and dynamic optimal control problems (see Roberts (2001) and the references quoted therein). The main characteristic is that it is an iterative method which converges to the correct optimum condition in spite of model-reality differences. In this paper, after deriving a general ISOPE algorithm for on-line steady-state optimisation, the main emphasis is to demonstrate it's application to a significant and realistic benchmark case study.

2. STEADY-STATE PROBLEM FORMULATION

The steady-state behaviour of the regulated industrial process in Figure 1 may be represented as:

$$y^* = f^*(v) \qquad (1)$$

where $v \in \Re^{n_c}$ and $y^* \in \Re^{n_y}$ are the applied controller set points and resulting process steady-state outputs respectively, and $f^* : \Re^{n_c} \to \Re^{n_y}$ represents the real process steady-state input-output mapping. In general the controller set points will be limited and the outputs will be constrained as represented by:

$$v_{\min} \le v \le v_{\max} \qquad (2)$$

$$g(y^*, v) \le 0 \qquad (3)$$

The steady-state performance of the process is expressed as:

$$J^* = J^*(y^*, v) \qquad (4)$$

and thus the real optimisation problem, ROP, expressed in terms of computing set points v to minimise J^*, while satisfying constraints defined by Equations (2) and (3), can be expressed as:

$$\left\{ \begin{array}{l} \min\limits_{v,y^*} J^*(y^*, v) \\ \text{subject to } y^* = f^*(v),\ v_{\min} \le v \le v_{\max} \\ \qquad g(y^*, v) \le 0 \end{array} \right\} \qquad (5)$$

In a given situation the real process relationship, Equation (1), will not be known precisely. We then represent the real process mapping by an approximate model containing parameters whose values can be selected in an adaptive manner to match the model to the real process. Also, to separate the real situation from the model we use symbol c for the set points to be calculated from the model-based optimisation problem and then employ the equality

$$v = c \qquad (6)$$

within an updating mechanism. The model of Equation (1) is:

$$y = f(c, \alpha) \qquad (7)$$

where $\alpha \in \Re^{n_\alpha}$ is the vector of model parameters, estimated by satisfying the matching equality

$$f(v, \alpha) = f^*(v) \qquad (8)$$

after every application of set points v.

In addition, instead of operating on $J^*(y^*,v)$ in ROP defined by Equation Group (5), we choose to operate on a different performance index $J(y^*,v,\gamma)$ where $\gamma \in \Re$ is a scalar parameter which can be estimated by satisfying the equality

$$J(y^*, v, \gamma) = J^*(y^*, v) \qquad (9)$$

By this means it is possible to replace a realistic practical but, perhaps, complicated performance index with a simpler one that is mathematically tractable. Hence, model-reality differences now occur in the performance index $J^*(y^*,v)$ as well as in the system representation $f^*(v)$. Note that the aim is still to design an iterative scheme to determine the set-points v which solve the real optimisation problem ROP defined by Equation Group (5).

The key to achieving this aim is to replace Equation Group (5) by the equivalent problem EOP

$$\left\{ \begin{array}{l} \min\limits_{c,y,\gamma} J(y, c, \gamma) + r\|v - c\|^2 \\ \text{subject to } y = f(c, \alpha),\ c_{\min} \le c \le c_{\max} \\ \qquad g(y, c) \le 0,\ \ v = c \\ \qquad y^* = f^*(v) \\ \qquad f(v, \alpha) = f^*(v) \\ \qquad J(y^*, v, \gamma) = J^*(y^*, v) \end{array} \right\} \qquad (10)$$

where the scalar $r \ge 0$ is a positive weighting parameter introduced to improve convexity (Brdyś *et al*, 1987).

The solution of EOP given by Equation Group (10) is determined from optimality conditions corresponding to the Lagrangian

$$\begin{aligned} L(.) = {} & J(y, c, \gamma) + \tfrac{1}{2} r\|v - c\|^2 + \lambda^T (v - c) \\ & + \mu^T \left(y - f(c, \alpha) \right) + \sigma^T g(y, c) + \sigma_-^{\ T} (c_{\min} - c) \\ & + \sigma_+^{\ T} (c - c_{\max}) + \eta^T \left(f^*(v) - f(v, \alpha) \right) \\ & + \zeta \left(J^*(y^*, v) - J(y^*, v, \gamma) \right) + \beta^T \left(y^* - f^*(v) \right) \end{aligned} \qquad (11)$$

where $\lambda \in \Re^{n_c}$, $\mu \in \Re^{n_y}$, $\eta \in \Re^{n_y}$, $\zeta \in \Re$ and $\beta \in \Re^{n_y}$ are Lagrange multipliers, $\sigma \in \Re^{n_y}$, $\sigma_- \in \Re^{n_c}$ and $\sigma_+ \in \Re^{n_c}$ are Kuhn-Tucker multipliers. Investigating the first order necessary optimality conditions (Roberts, 2001) shows that they can be satisfied by solving the following modified model-based optimisation problem MMOP:

$$\left\{ \begin{array}{l} \min\limits_{c,y} J(y, c, \gamma) + \tfrac{1}{2} r\|v - c\|^2 - \lambda^T c \\ \text{subject to } y = f(c, \alpha),\ c_{\min} \le c \le c_{\max} \\ \qquad g(y, c) \le 0 \end{array} \right\} \qquad (12)$$

under given v, λ, α and γ, where α and γ are model parameters which can be obtained from Equations (1), (8) and (9) at a given v. The Lagrange multiplier λ, henceforth termed the modifier, is determined from

$$\lambda = -\left[\frac{\partial f^*(v)}{\partial v} - \frac{\partial f(v, \alpha)}{\partial v} \right]^T \left(\nabla_y J(y, v, \gamma) \right.$$

$$+\left[\frac{\partial g(y,v)}{\partial y}\right]^T \sigma \Bigg) - \left(\nabla_v J^*(y^*,v) - \nabla_v J(y^*,v,\gamma)\right)$$

$$-\left[\frac{\partial f^*(v)}{\partial v}\right]^T \left(\nabla_{y^*} J^*(y^*,v) - \nabla_{y^*} J(y^*,v,\gamma)\right) \quad (13)$$

at a given v. Note that the Kuhn-Tucker multiplier σ is also required when Equation (13) is employed to compute λ.

3. ISOPE ALGORITHM

The modified model-based optimisation problem MMOP, given by Equation Group (12), and modifier computation, given by Equation (13), are important constituents of an iterative scheme designed to satisfy the above optimality conditions. An appropriate algorithm is given as follows

Data:- model relationship $f(c,\alpha)$, model performance index $J(y,c,\gamma)$, real performance index $J^*(y^*,v)$, and coefficients r, k_v and k_σ.

Step 0 *Initialisation*:-Select an initial vector of set-points $v^{(0)}$ and Kuhn-Tucker multiplier vector $\sigma^{(0)}$. Set iteration counter $i = 0$.

Step 1 *Parameter estimation*:- Apply set-point vector $v^{(i)}$ to the real process. Wait a sufficient time for dynamic transients to decay and then measure the real steady-state outputs $y^{*(i)}$, thus effectively implementing Equation (1). Then compute the parameters $\alpha^{(i)}$ and $\gamma^{(i)}$ to satisfy Equations (8) and (9).

Step 2 *Modifier Computation*:- Use Equation (13) to compute the modifier vector $\lambda^{(i)}$.

Step 3 *Modified Optimisation*:- Determine model set-point vector $c^{(i)}$ and Kuhn-Tucker multiplier estimate $\hat{\sigma}^{(i)}$ by solving the modified model-based optimisation problem MMOP given by Equation Group (12).

Step 4 *Update*:- Use the following relaxation scheme to update $v^{(i)}$, and $\sigma^{(i)}$.

$$\begin{Bmatrix} v^{(i+1)} = v^{(i)} + k_v\left(c^{(i)} - v^{(i)}\right) \\ \sigma^{(i+1)} = \sigma^{(i)} + k_\sigma\left(\hat{\sigma}^{(i)} - \sigma^{(i)}\right) \end{Bmatrix} \quad (14)$$

Then repeat from *Step 1* until convergence is achieved.

This algorithm is also known as the modified two-step approach where the modification consists of the additional linear term $-\lambda^T c$ in the performance index of the modified model-based optimisation problem. The two steps refer to repeated solution of the modified optimisation problem followed by parameter estimation. This additional term compensates for inevitable model-reality differences and is essential if the iterations are to converge to a correct solution of the real optimisation problem, ROP, defined by Equation Group (5).

3.1 Convergence considerations

A full analytical analysis of the convergence properties of the ISOPE algorithm in its full form described above has not yet been performed. However, by comparison with previous analysis of more basic ISOPE algorithms without performance index model-reality differences, it is expected that convergence performance will be enhanced if the overall problem is at least locally convex (Brdyś *et al*., 1987). In the practical implementation of the algorithm relaxation gains, k_v and k_σ and convexification term coefficient r are provided in order to regulate stability and convergence.

3.2 Derivative acquisition

It is observed from Equation (13) that several derivative information sets need to be computed in order to compute the modifier vector λ. All except one are model based, or are analytic in terms of known constraints and performance indices, and can readily be computed. The exception is $\partial f^*(v)/\partial v$, which requires real process derivative information. Clearly there will be practical difficulties in obtaining reliable estimates of the real process derivatives and this is a significant limitation to the on-line ISOPE technique. Early versions of the ISOPE technique used finite difference techniques to obtain the real derivatives by applying perturbations to y^*. The finite difference method is particularly costly because it requires an additional steady-state detection for each controller set point at each iteration, significantly slowing down the rate at which the iterations progress towards the optimum. However, employing results of consecutive applications of set-points to estimate the required derivatives can reduce this cost. This has been formulated rigorously within a specially designed ISOPE technique employing a dual optimising algorithm, resulting in a powerful method for on-line steady-state optimisation (Brdyś and Tatjewski, 1994). The Broyden technique (Broyden, 1965) also offers a method for estimating the required derivatives and has been incorporated successfully within both steady-state and dynamic ISOPE algorithms (Roberts, 2000).

Some ISOPE algorithms, based on work by Bamberger and Isermann (1978), use dynamic perturbation and linear system identification methods to estimate the derivatives (Zhang and Roberts, 1990) and this has been applied in an industrial application of the ISOPE method (Griffiths, et al, 1994). This method estimates the derivatives of the real process mapping with respect to the manipulated variables by identifying a dynamic model on-line and reducing it to a steady state model. In this work, a multivariable ARMAX model with the following structure is identified:

$$y(k) = -A_1 y(k-1) - \cdots - A_{n_A} y(k-n_A)$$
$$+B_1 v(k-1) + \cdots + B_{n_B} v(k-n_B)$$
$$+\varepsilon(k) + C_1\varepsilon(k-1) + \cdots + C_{n_C}\varepsilon(k-n_C) + \overline{c} \quad (15)$$

where $\varepsilon \in \Re^{n_y}$ is assumed to be zero mean white noise, k is a discrete time index, A_i, B_i, C_i are matrix coefficients of the appropriate dimensions, and $\overline{c} \in \Re^{n_y}$ *is* an off-set vector.

The identification algorithm used in this work is a multivariable moving horizon least squares based method (Becerra *et al*, 1998). Note that it is often necessary to add small perturbation signals to the manipulated variables, such that the inputs are sufficiently exciting and a model can be estimated from the measured data. Also notice that it is possible to enhance the model fit at low frequencies by filtering the data using a low pass filter (Ljung, 1987).

A static model is obtained by assuming that outputs y and inputs v are at steady state, and that the noise ε is zero. This gives the following linear input-output relationship:

$$y = \left[I_{n_y} + A_1 + \cdots + A_{n_A} \right]^{-1} \left[B_1 + \cdots + B_{n_B} \right] v + \overline{c}$$
$$= Gv + \overline{c} \quad (16)$$

and thus G is the estimate of $\partial y^*(v) / \partial v$.

3.3 *Case with linear-quadratic model based optimisation*

A particular case arises when the model relationship *f*(.), constraints *g*(.) are both linear, and the performance index *J*(.) is quadratic, all as defined in Equation Group (12). Then the modified model-based optimisation problem MMOP is a quadratic programming problem for which standard procedures are available (Gill *et al*, 1984). For instance, if

$$y = f(c,\alpha) = Ac + \alpha \quad (17)$$

$$J(y,c,\gamma) = \tfrac{1}{2}\left((y-y_d)^T Q (y-y_d) + c^T Rc \right)$$
$$+q^T y + s^T c + \gamma \quad (18)$$

where A, Q R q and s are matrices or vectors of appropriate dimensions ($Q \geq 0$, $R > 0$), and y_d is a reference steady-state output vector, the unconstrained solution of MMOP is analytic, given by

$$c = \left[\overline{R} + A^T QA \right]^{-1} \left(A^T Q (y_d - \alpha) \right.$$
$$\left. -A^T q - s + \lambda + rv \right) \quad (19)$$

where

$$\overline{R} = R + rI_{n_c} \quad (20)$$

The solution of the parameter estimation problem defined by Equation (8) then becomes

$$\alpha = f^*(v) - Av \quad (21)$$

and there is no requirement to determine parameter vector γ. Furthermore, when the equality constraints are output-independent, the expression for the modifier defined by Equation (13) becomes

$$\lambda = -\left[\frac{\partial f^*(v)}{\partial v} - A \right]^T \left(Q(Av + \alpha - y_d) + q \right)$$
$$-\left(\nabla_v J^*(y^*, v) - Rv - s \right)$$
$$-\left[\frac{\partial f^*(v)}{\partial v} \right]^T \left(\nabla_{y^*} J^*(y^*, v) - Q(y^* - y_d) - q \right) \quad (22)$$

Since, after parameter estimation, $y^* = Av + \alpha$, Equation (22) further simplifies to

$$\lambda = A^T \left(Q(y^* - y_d) + q \right) - \left(\nabla_v J^*(y^*, v) - Rv - s \right)$$
$$-\left[\frac{\partial f^*(v)}{\partial v} \right]^T \nabla_{y^*} J^*(y^*, v) \quad (23)$$

4. APPLICATION TO THE TENNESSEE EASTMAN PROCESS

The Tennessee Eastman process model consists of a reactor, condenser, separator, compressor and stripper with a gas recycle stream. This model was proposed as a plant-wide control test problem (Downs and Vogal, 1993). The process produces two products from four reactants. There are two main exothermic reactions:

$$\tilde{A} + \tilde{C} + \tilde{D} \rightarrow \tilde{G} \quad (24)$$
$$\tilde{A} + \tilde{C} + \tilde{E} \rightarrow \tilde{H} \quad (25)$$

Two additional irreversible and exothermic side reactions produce by-product $\tilde{F}$. The reactor, which is open loop unstable, has both liquid and vapour phases, but only a gas stream leaves the reactor. The vapour stream from the reactor passes through a partial condenser and then into a separator drum. Liquid from the drum is fed to the stripping column. A small proportion of the vapour stream, which leaves the separator drum, is purged and the rest is compressed and recycled back to the reactor. The reactor has an internal cooling bundle for removing the heat of reaction. The stripper has two sources of vapour: a reboiler and the $\tilde{C}$ feed stream. Further details listing 41 measured variables and 12 manipulated variables are given in Becerra and Roberts (2000).

The objective for economic optimisation is to minimise operating costs in *$/h*. The equation for the operating cost is a linear function of the output measurements.

$$J(X) = J_1(X) + J_2(X) + J_3(X) \quad (26)$$

where X is the vector of process measurements (41 in total), $J_1(X)$ is the compressor and stripper steam costs:

$$J_1(X) = 0.0536X_{20} + 0.0318X_{19} \quad (27)$$

$J_2(X)$ represents the purge losses:

$$J_2(X) = 0.4479X_{10}\left(2.206X_{29} + 6.177X_{31} + 22.06X_{32} + 14.56X_{33} + 17.89X_{34} + 30.44X_{35} + 22.94X_{36}\right) \quad (28)$$

and $J_3(X)$ represents the product losses

$$J_3(X) = 0.0921X_{17}\left(22.06X_{37} + 14.56X_{38} + 17.89X_{39}\right) \quad (29)$$

4.1 Control structure

The regulatory control structure used in this work is based on one of the structures given in Luyben *et al* (1998), where it is assumed that the flow rate of the product stream leaving the base of the stripper is set by a downstream customer. This base control consists of controllers for levels (reactor, separator and stripper), reactor pressure, temperatures (reactors, separator and stripper), compositions (composition of $\tilde{B}$ in purge and composition of $\tilde{A}$ in the reactor feed), $\tilde{G}/\tilde{H}$ ratio and product flow (see Becerra and Roberts (2000) for further details). The separator temperature controller provides the set point to the reactor temperature controller, in a cascade configuration.

The structure of the optimising controller consists of 5 set point variables and 6 process measured variables, including the operating cost. The variables and constraints used by the optimiser are shown in Becerra and Roberts (2000). Other important parameters are: ARMAX model orders: n_A = 1, n_B = 4, n_C = 0; identifier sampling time: 6 min.; identifier data length: 120 points; optimiser updating period: 2 hours; optimiser relaxation gain k_v: 0.1; optimiser convexification factor r: 0.0; optimiser penalty factor ρ: 100.0 (used in the treatment of output dependent constraints as soft constraints incorporated as a penalty function (Becerra and Roberts, 2000)). A pseudo random binary sequence was added to each manipulated variable to enhance input excitation and allow the identification of an accurate model. Since the cost J given in Equation (26) is included as an output of the identified model, then the objective function is $J = y_6$, which reflects the objective of minimising the operational cost J.

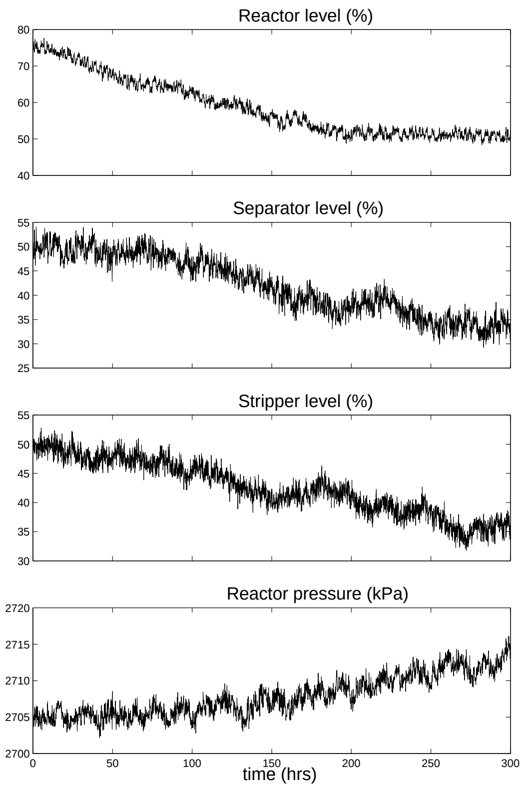

Fig. 2. Simulation results: levels and reactor pressure

4.2 Results

The initial value of the economic cost is 170.6 \$/hour. Figures 2 and 3 show the simulation results for the dependent variables. Notice in Figure 3 how the economic cost decreases to around 120 \$/hour after about 250 hours. Figure 4 shows the trajectories of the manipulated controller set points. Notice how the three level set points involved in the optimisation (reactor, stripper and separator) reduce their values, and how the reactor pressure and $\tilde{B}$ purge composition set points both increase during the simulation.

The final cost value of 120 \$/hour may be compared to the optimum value reported by Ricker (1995) of 114 \$/hour. The value reported by Ricker may be considered to be the absolute optimum for this operating condition ($\tilde{G}/\tilde{H}$ ratio by mass 50/50), since, unlike in this work, only the noise free steady state part of the model was used and all manipulated variables were adjusted directly (no regulatory control was

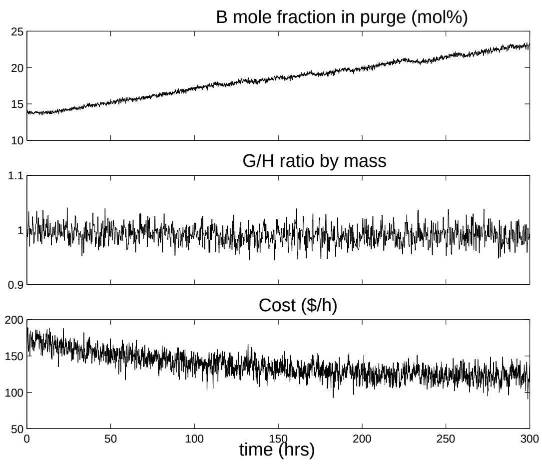

Fig. 3. Simulation results: $\tilde{B}$ mole fraction in purge, $\tilde{G}/\tilde{H}$ ratio and cost.

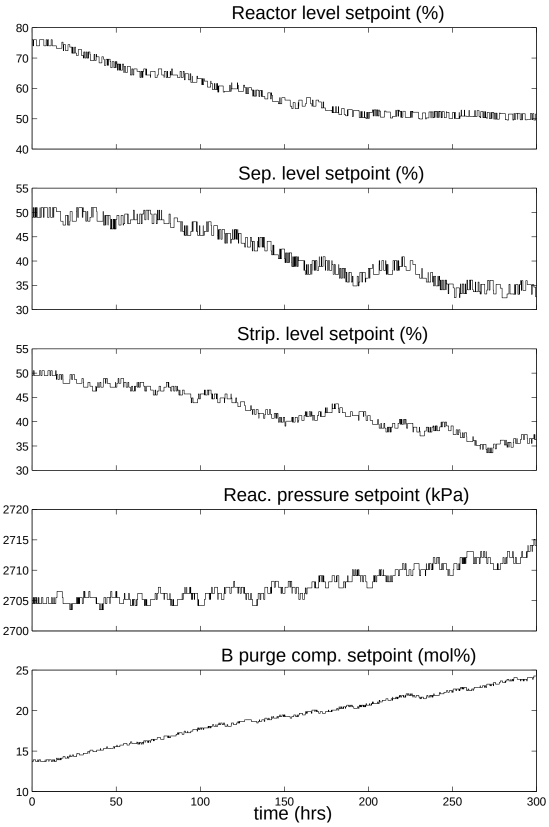

Fig. 4. Simulation results: manipulated set points.

considered). The result obtained in this work can be considered to be the optimum for the regulatory control and set point manipulated variables used.

5. CONCLUSIONS

An advantage of the ISOPE technique is that a rigorous model is not required within the hierarchical optimisation scheme. It has been shown that effective on-line steady-state optimisation can be achieved using a simple linear model and quadratic model performance even when the real situation is non-linear with a non-quadratic performance. The utility of the approach has been successfully demonstrated using a realistic simulation study of the Tennessee Eastman process. In particular, it has been demonstrated that real process derivatives required by the ISOPE technique can be effectively obtained using dynamic identification.

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