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ADAPTIVE CONTROL OF A NEUTRALIZATION REACTOR

José Figueroa and Juan Cousseau^{*,1} Stefan Werner and Timo Laakso^{**}

* Departamento de Ingeniería Eléctrica y de Computadoras, Universidad Nacional del Sur, Av. Alem 1253; (8000) Bahía Blanca, Argentina
** Signal Processing Laboratory, Smart and Novel Radios (SMARAD) Center of Excellence, Helsinki University of Technology, P.O. BOX 3000, FIN-02015 HUT, Finland

Abstract: In this paper the problem of on-line identification and adaptive control of Neutralization reactor is studied. It is used the fact that this process can be modeled as a Wiener type system. An recursive identification algorithm for Wiener systems is proposed whose linear and nonlinear parts are modeled using a Laguerre and Piecewise Linear basis functions, respectively. The model obtained is used to adapt the parameters of a controller designed for the specific structure of the model. The results show good performance when compared with other similar schemes found in the literature.

Keywords: Adaptive filtering, Nonlinear control, Adaptive Control.

1. INTRODUCTION

In the last decades, many contributions for controller design have been based on the linear model assumption. However, in some cases it is difficult to represent a given process using a linear model. This is the case when the system is highly nonlinear and the operating point changes along a wide region, or when the process is nonstationary, i.e., the characteristics change with time.

In these cases, the controller design can be performed using special techniques, such as exact linearization, nonlinear model predictive control, or other special purpose procedures (Ogunnaike and Ray, 1994).

One of the solutions to control such kind of systems is *adaptive control*, where the parameters

of a linear controller are adjusted to follow the variations of the process behavior. Several control schemes assume a model structure whose parameters are identified on-line using an adaptive identification algorithm. The identified model parameters are then used to adjust the controller parameters.

It is well known that some systems can be described by a linear dynamic model followed by a static nonlinearity, i.e., a *Wiener system* (Pearson and Pottmann, 2000; Pearson, 2003). In this paper, an algorithm for adaptive control for Wiener models is presented.

The first step in the construction of an adaptive control algorithm is to obtain an efficient adaptive identification scheme. In this paper we use the identification methodology of block-oriented models introduced by Bai (1998). The algorithm is based on least-squares estimation (LSE) and singular value decomposition (SVD). The approach

 $^{^1}$ Corresponding author. Email: figueroa@uns.edu.ar. Phone: +54 291 4595101 ext. 3325. FAX: +54 291 4595154.

is useful only for the single input/single output (SISO) case due to the particular parameterization used. Gómez and Baeyens (2004) extended the results of Bai to include a more general parameterization that enables the use of multiple input/ multiple output (MIMO) systems.

In this paper we propose a new approach for adaptive control of Wiener type systems. In particular we propose the use of a Laguerre description for the linear part and a Piecewise Lineal description for the nonlinear gain. For this parametrization, an adaptive identification scheme is proposed extending the idea of Gómez and Baeyens (2004). Using this approach, the inverse of the nonlinearity is directly identified, avoiding the inversion problem. After that, the structure of the Wiener model is fully exploited to obtain all possible advantages.

The performance of the proposed algorithm is tested in the control of a neutralization reactor. It is well known that the control of a pH processes is particularly difficult. The main reason is the strong nonlinearity involved. The slope of a chemical system's titration curve can vary several orders of magnitude over a modest range of pH values, causing the overall process gain to change accordingly. The control of this kind of processes can be performed by several nonlinear schemes (Norquay et al., 1998; Norquay et al., 1999; Gerkšič et al., 2000; Lussón et al., 2003a; Biagiola et al., 2004; Akesson et al., 2005). The basic assumptions of these schemes are a fixed Wiener structure of the model and a fixed nonlinear controller. Several control strategies were used (including gain scheduling, model predictive control, H_{∞} , etc.).

However, when perturbations are applied to the process, a fixed Wiener model does not longer represents adequately the process. For example, the titration curve change drastically (Kalafatis et al., 2005b). These move to some authors to include some robustness ideas in the controller design (Lussón et al., 2003b), to use feedforward controllers (Kalafatis et al., 2005b) or to use adaptive identification algorithms (Kalafatis et al., 2005a). Pajunen (1987 and 1992) propose two adaptive control schemes for the control of Wiener systems. However, in the identification algorithms of these schemes, the Wiener structure is lost, resulting in a large number of parameters for the process model. In this paper we propose, as mentioned above, a more efficient algorithm to solve for adaptive control.

The paper is organized as follows. In Section 2 a description of model structure and adaptive identification procedure are presented. Section 3 describes the adaptive control algorithm and discusses some implementation details. A simulation example describing the application of this algo-



Fig. 1. Laguerre-PWL Wiener Model.

rithm to control a pH neutralization reactor is detailed in Section 4. Finally, in Section 5 the conclusions are presented.

2. ADAPTIVE IDENTIFICATION SCHEME

2.1 Model Description

We propose in this paper a special description for the process, where the linear dynamic model is described by a Laguerre basis series and the nonlinear static block is modeled as a Piecewise Linear (PWL) model. This model is illustrated in Fig. 1. The Laguerre basis allows the use of prior knowledge about the dominant poles (Wahlberg, 1991; 1994; Lindskog, 1996). This model describes the linear model with the following basis function expansion

$$H(z) = \sum_{i=0}^{M} h_i L_i(z, a) \tag{1}$$

where

$$L_i(z,a) = \frac{\overline{1-a^2}}{z-a} \left(\frac{1-az}{z-a}\right)^{i-1}$$
(2)

and h_i are the parameters of the model, a is a filter coefficient chosen a priori (Wahlberg, 1991).

For the representation of the static nonlinear gain, $N(\cdot)$, we use a Piecewise Linear (PWL) description. In general $N(\cdot)$ is a real-valued function of one variable, i.e., y = N(v): ¹ ¹, which we will assume to be invertible. This is a common assumption in the adaptive identification area (Wigren, 1994), often to allow a simplification in the feedback loop design (Lussón *et al.*, 2003*a*). For the specific control algorithm that we will use, we prefer to describe the inverse of this nonlinearity, i.e., $v = N^{-1}(y)$.

PWL functions have proven to be a very powerful tool in the modeling and analysis of nonlinear systems (Chua and Ying, 1983; Julián *et al.*, 1999). It can be proved (Julián *et al.*, 1999) that any continuous nonlinear function f(v): m 1 can be uniquely represented using PWL functions. To express the nonlinear function, we will use a function expansion with basis functions and parameters

$$v = \mathbf{c}^T \mathbf{\Lambda}(y). \tag{3}$$

We will consider the case where the basis functions that are included in the matrix Λ have been predetermined, and the values of **c** are the parameters to be estimated. In this paper we use the orthogonal basis description proposed by Julián *et al.* (2000).

Since the basis functions Λ are fixed, the output is a linear function of the parameters. This allows us to use linear regression to estimate these parameters. The two basic advantages of this approach are its fast convergence and unique solution.

2.2 Adaptive implementation

Let us define an adaptive algorithm for the identification of the Wiener model described in previous section. As can be seen from Fig. 1, the signal v(k) is given by

$$v(k) = \sum_{i=0}^{M} h_i L_i[u(k)]$$
 (4)

and also

$$v(k) = N^{-1}[y(k)] = \mathbf{c}^T \mathbf{\Lambda}[y(k)]$$
$$= \sum_{i=0}^N c_i \Lambda_i[y(k)]$$
(5)

By equaling both sides of (4) and (5) (including $\epsilon(k)$ to allow a modeling error), and fixing the parameter $h_0 = 1$ to overcome the well-known gain ambiguity in Wiener models, the following equation is obtained

$$\epsilon(k) = \sum_{i=0}^{N} c_i \Lambda_i[y(k)] - L_0[u(k)] - \sum_{i=1}^{M} h_i L_i[u(k)] = \boldsymbol{\theta}^T(k) \boldsymbol{\phi}(k) - L_0[u(k)] \quad (6)$$

where vectors $\boldsymbol{\theta}(k)$ and $\boldsymbol{\phi}(k)$ are defined as

$$\boldsymbol{\theta}(k) = [c_0, c_1, c_2, \cdots, c_N, h_1, h_2, \cdots, h_M]^T \quad (7)$$

$$\phi(k) = [\Lambda_0[y(k)], \Lambda_1[y(k)], \dots, \Lambda_N[y(k)], -L_1[u(k)], -L_2[u(k)], \dots, -L_M[u(k)]]^T.$$
(8)

Next, we consider an stochastic gradient algorithm to estimate recursively the parameters of the model $\boldsymbol{\theta}$. For this purpose, we use as objective function $J_{\boldsymbol{\theta}}$, the instantaneous squared error, i.e.

$$J_{\boldsymbol{\theta}}[\epsilon(k)] = \epsilon^2(k) = \left[\boldsymbol{\theta}^T(k)\boldsymbol{\phi}(k) - L_0[u(k)]\right]^2$$
(9)

The recursion of the stochastic gradient algorithm that minimizes the above objective function is given by

$$\boldsymbol{\theta}(k+1) = \boldsymbol{\theta}(k) + \mu \boldsymbol{\phi}(k) \boldsymbol{\epsilon}(k). \tag{10}$$

where μ is the step size controlling the convergence and final error of θ . A bound on μ to ensure convergence and an analysis of convergence to a local stationary point can be found in Figueroa *et al.* (2004).

The identification algorithm is summarized in Table 1. From the implementation point of view, the initial condition for h is the vector zero and for c is the parameters that defines the identity nonlinear function.

Table 1. The adaptive identification algorithm.

Parameters:
M = number of h coefficients
N = number of c coefficients
$\mu = \text{step size}$
Data:
u(k) input signal at time k
y(k) output signal at time k
Initialization
h(0) = 0
$\boldsymbol{c}(0) = [-1 \ 1 \ 0 \ \cdots \ 0 \ -1]^T$
For each k ,
$\boldsymbol{\theta}(k) = [c_0, \cdots, c_N, h_1, \cdots, h_M]^T$
$\boldsymbol{\phi}(k) = [\Lambda_0[y(k)], \cdots,$
$\Lambda_N[y(k)], -L_1[u(k)], \cdots, -L_M[u(k)]]^T$
$\boldsymbol{\epsilon}(k) = \boldsymbol{\theta}^T(k)\boldsymbol{\phi}(k) - L_0[u(k)]$
$\boldsymbol{\theta}(k+1) = \boldsymbol{\theta}(k) + \mu \boldsymbol{\phi}(k) \boldsymbol{\epsilon}(k)$

3. CONTROLLER DESIGN

In the context of adaptive control, the essential idea is to identify a process and, based on the model obtained, adjust the controller parameters to improve the closed loop performance. For tuning the control parameters any classical strategy could be used, for example: minimum ITAE, retain constant loop gain, Ziegler-Nichols, Cohen-Coon, internal model control, etc. (Ogunnaike and Ray, 1994). In our particular application, we used a direct synthesis approach, which was modified to be applied to a Wiener model.

To design the controller, we will follow the principle of the nonlinear regulator as presented by Wigren (1999). Consider the closed-loop system of Fig. 2. The process is assumed to be represented by a Wiener model with a nonlinear gain $N(\cdot)$ that is invertible. We can use the inverse of this



Fig. 2. The closed loop scheme for known Wiener Model.

block to extract the nonlinearities outside of the closed loop. In this way, a linear controller K(z) should be designed to compensate the behaviour of the linear dynamic block of the process model.

In our case, the inverse of the nonlinearity is obtained directly from the identification process. To design the linear controller, we adopt the direct synthesis approach (Ogunnaike and Ray, 1994), applied to the Laguerre model of Eq. (4). The controller specification is to obtain a closed-loop pole in a_c without offset when the set point is changed in the form of steps. If the discrete transfer function of the linear model is called H(z), and $H^{-1}(z)$ is stable and causal, then the controller can be defined as

$$K_{\boldsymbol{h}}(z) = \frac{a_c}{z - 1} \frac{1}{H(z)}.$$
(11)

where the subscript h is included to remark the dependence of the controller with the parameters of the Laguerre model. The control algorithm is summarized in Table 2. A stability analysis for the fixed controller is similar to the one presented in Biagiola *et al.* (2004).

Table 2. The control algorithm.

Parameters:
Coefficients of Laguerre model h .
Coefficients of PWL model \boldsymbol{c} .
Data:
$y_r(k)$ set point at time k
For each k ,
Obtain $y(k)$ as measure from the process
Compute $v(k) = \mathbf{c}^T \mathbf{\Lambda}[y(k)]$
Compute $v_r(k) = \mathbf{c}^T \mathbf{\Lambda}[y_r(k)]$
Compute $e(k) = v_r(k) - v(k)$
Compute $u(k)$ by applying $e(k)$ to $K_{\mathbf{h}}(z)$
Applied $u(k)$ to the process.

Let us now consider the problem of controlling the process when the parameters of the Wiener model are unknown and varying along the operation. We can use the adaptive identification algorithm in Section 2 to obtain the parameters of the model, and use them to adapt the controller coefficients. This implies that each sample time, both algorithms (Table 1 and Table 2) are executed simultaneously. The complete adaptive scheme is illustrated in Fig. 3. The dotted lines denote the parameter information flow from the identification scheme to the compensator. In this formulation, the role of the measurement noise is essential in order to ensure the persistent excitation.



Fig. 3. The control adaptation scheme.

In the next section, this scheme is applied to the control of a pH neutralization reactor.

4. EXAMPLE: PH NEUTRALIZATION

In order to illustrate the design procedure and to evaluate the adaptive controller performance, simulation results were obtained. A chemical process with strong nonlinearity was selected. The example consists of the neutralization reaction between a strong acid (HA) and a strong base (BOH) in the presence of a buffer agent (BX)as described by Galán (2000). The neutralization takes place in a continuous stirred tank reactor (CSTR) with a constant volume V.

It is well known that the control of a pH processes is particularly difficult. The main reason is the high nonlinearity involved. The slope of the titration curve of the chemical system can vary several orders of magnitude over a modest range of pH values, causing the overall process gain to change accordingly. The regions of high and low slope on the titration curve correspond to conditions of high and low gain for a pH control loop, respectively.

In the continuous pH neutralization reactor an acidic solution, with a time-varying volumetric flow $q_A(t)$ of a composition $x_{1i}(t)$, is neutralized using an alkaline solution with volumetric flow $q_B(t)$ of known composition made up of base x_{2i} and buffer agent x_{3i} . Due to the high reaction rates of the acid-base neutralization, chemical equilibrium conditions are instantaneously achieved. Moreover, assuming that the acid, the base and the buffer are strong enough, the total dissociation of the three compounds takes place.

The process dynamics model can be obtained by considering the electroneutrality condition (which is always preserved) and through mass balances of equivalent chemical species (known as chemical invariants) that were introduced by Gustafsson and Waller (1983). For this specific case, under the previous assumptions, the dynamic behavior of the process can be described considering the following state variables:

$$x_1 = [A^-] \tag{12}$$

$$x_2 = [B^+] \tag{13}$$

$$x_3 = [X^-] \tag{14}$$

Therefore, the mathematical model of the process can be written in the following way (Galán, 2000):

$$\dot{x}_1 = 1/\eta (x_{1i} - x_1) - 1/V x_1 q_B$$
 (15)

$$\dot{x}_2 = -1/\eta \ x_2 + 1/V \ (x_{2i} - x_2)q_B \ (16)$$

$$\dot{x}_3 = -1/\eta \, x_3 + 1/V \, (x_{3i} - x_3)q_B \quad (17)$$

$$F(x,\xi) \quad \xi + x_2 + x_3 - x_1 - K_w / \xi - x_3 / [1 + (K_x \xi / K_w)] = 0 \quad (18)$$

where $\xi = 10^{-pH}$ and $\theta = V/q_A$. K_w and K_x are the dissociation constants of the buffer and the water, respectively. Note that this process is not strictly a Wiener process, however, it will be use to illustrate the proposed control. The parameters of the system represented by Eq. (15)–(18) are addressed in Table 3. Eq. (18) was deduced by McAvoy *et al.*, (1972) and takes the standard form of the widely used implicit expression that connects the pH value with the states of the process.

Table 3. Neutralization Parameters.

PARAMETER	VALUE
x_{1i}	$0.0012 \ mol \ HCL/l$
x_{2i}	$0.0020 \ mol \ NaOH/l$
x_{3i}	$0.0025 \ mol \ NaHCO_3/l$
K_x	$10^{-7} \ mol/l$
K_w	$10^{-14} \ mol^2/l^2$
q_A	1 l/m
V	$2.5 \ l$

A Wiener model describing this process has been presented for several control applications using q_B (manipulated variable) to control the pH (controlled variable), see, e.g., Lussón *et al.* (2003*a*) and Biagiola *et al.* (2004). However, when perturbations are present in the process ($q_A(t)$ and $x_{1i}(t)$), a simple Wiener model cannot provide an adequate representation of the plant.

The chosen parameters for our model are a thirdorder Laguerre basis with a pole at a = 0.7 to represent the linear dynamic model, /it i.e. M =2. To represent the inverse of the nonlinear gain, the domain of the pH, the range [3, 9.5], is divided in 10 regions, /it i.e. N = 11. The adaptation step size is $\mu = 0.015$.

In this particular application, the linear controller takes the form

$$K(z) = \frac{a_c \left(z^3 - 3az^2 + 3a^2z - a^3\right)}{1 - a^2 \left(a_2 z^2 + a_1 z + a_0\right) \left(z - 1\right)} (19)$$

where $a_2 = 1 - ah_2 + a^2h_3$, $a_1 = h_2 - 2ah_3 + a^2 - 2a$, $a_0 = h_3 - ah_2 + a^2$ and the closed-loop pole is fixed at $a_c = 0.8$. In the adaptive adjustment of this controller, it is important to check the stability at every iteration. If a pole is outside the unit circle, it should be replaced by its stable reciprocal.



Fig. 4. Simulation results. y = pH as function of time.



Fig. 5. Simulation results. $u = q_b$ as function of time.

Now, the results of the proposed adaptive controller are presented, and the performance is compared with that of the Model Reference Adaptive Technique proposed by Pajunen (1992).

The simulation involve a set point change from $pH_1 = 7.7182$ to $pH_2 = 9.7182$ at $t_2 = 25min$ and to $pH_3 = 5.7182$ at $t_3 = 100min$. Perturbations are applied in q_A (which is increased from 1 to 1.2 at t = 38min and then reduced to 0.8 at t = 113min) and in x_{1i} (which increases 10 percent from the original value at t = 63min and then is reduced 20 percent at t = 138min). In all cases a uniform noise in the range of ± 0.05 is considered.

Figure 4 illustrates the pH behaviour of the controllers. From this plot it is clear that the performance of the proposed Laguerre-PWL Wiener adaptive controller is better than the one proposed by Pajunen (1992). For example, our proposed remove completely the offset presented in the Pajunen scheme. Figure 5 depicts the manipulated variable q_B for the proposed algorithm.

An interesting point is to compare the number of the parameters involved in both approaches. While the identification of Laguerre-PWL involves 13 parameters, Pajunen's approach involves 23 parameters. This is because the Model Reference Adaptive Technique cannot take advantage of the Wiener structure of the model.

5. CONCLUSIONS

The problem of on-line identification and adaptive control of a neutralization reactor using a Wiener nonlinear system is studied. The linear and nonlinear parts are modeled using a Laguerre and Piecewise Linear basis functions, respectively. Then, since the fact that model error is linear in the parameters, an adaptive identification algorithm is presented based on a stochastic gradient algorithm. Information on the identified model is used to adjust the parameters of a controller online. The controller is designed based on the specific structure of the model. The complete scheme is successfully applied to a simulation example.

REFERENCES

- Akesson, B.M., H.T. Toivonen, J.B. Waller and R.H. Nyströn (2005). Neural network approximation of a nonlinear model predictive controller applied to a pH neutralization process. *Comp. and Chem. Eng.* 29, 323–335.
- Bai, E. (1998). An optimal two-stage identification algorithm for Hammerstein-Wiener nonlinear systems. Automatica 34, 3, 333–338.
- Biagiola, S.I., O.E. Agamennoni and J.L. Figueroa (2004). H_{∞} control of a wiener type system. Int. J. of Control **77**, **6**, 572–583.
- Chua, L.O. and L.P. Ying (1983). Canonical piecewise-linear analysis. *IEEE Trans. on Circuits and Systems* CAS-30, 125–140.
- Figueroa, J.L., J.E. Cousseau and R. J. P. de Figueiredo (2004). A simplicial canonical piecewise linear adaptive filter. *Circuits, Sys*tem and Signal Processing 23, 365–386.
- Galán, O. (2000). Robust multi-linear model-based control for nonlinear plants. PhD thesis. University of Sydney, Australia.
- Gerkšič, S., D. Juričic, S. Strmčnic and D. Matko (2000). Wiener model based nonlinear predictive control. *Int. J. of Systems Science* **31**, 189–202.
- Gómez, J.C. and E. Baeyens (2004). Identification of block-oriented nonlinear systems using orthonormal bases. J. of Process Control 14, 685–697.
- Gustafsson, T. and K. Waller (1983). Dynamic modelling and reaction invariant control of pH. Chem. Eng. Science 38, 389–398.
- Julián, P., A.C. Desages and M.B. D'Amicco (2000). Orthonormal high level canonical PWL functions with applications to model reduction. *IEEE Trans. on Circuits and Systems* CAS-47, 5, 702–712.
- Julián, P., A.C. Desages and O.E. Agamennoni (1999). High level canonical piecewise linear representation using a simplicial partition. *IEEE Trans. on Circuits and Systems* CAS-46, 463–480.

- Kalafatis, A., L. Wang and W.R. Cluett (2005a). Identification of time-varing ph processes using sinusoidal signals. Automatica 41, 385– 691.
- Kalafatis, A., L. Wang and W.R. Cluett (2005b). Linearizing feedforward-feedback control of pH processes based on the wiener model. J. of Process Control 15, 103–112.
- Lindskog, P. (1996). Methods, Algorithms and Tools for System Identification Based on Prior Knowledge. PhD thesis. Linköping Universitet, Sweden.
- Lussón, A., O. E. Agamennoni and J. L. Figueroa (2003a). A nonlinear model predictive control scheme based on Wiener piecewise linear models. J. of Process Control 13, 655–666.
- Lussón, A., O. E. Agamennoni and J. L. Figueroa (2003b). Robust identification of PWL-Wiener models: Use in model predictive control. Latin Am. App. Res. 33, 435–442.
- McAvoy, T., E. Hsu and S. Lowenthal (1972). Dynamics of pH in controlled stirred tank reactor. *Ind. Eng. and Chemistry Proc. Des. Dev.* **11**, **1**, 68–70.
- Norquay, S.J., A. Palazoglu and J.A. Romagnoli (1998). Model predictive control based on Wiener models. *Chem. Eng. Science* 53, 1, 75–84.
- Norquay, S.J., A. Palazoglu and J.A. Romagnoli (1999). Application of Wiener model predictive control (WMPC) to pH neutralization experiment. *IEEE Trans. Control System Technology* 7, 437–445.
- Ogunnaike, B.A. and W.R. Ray (1994). Process Dynamics, Modeling and Control. Oxford University. USA.
- Pajunen, G.A. (1987). Comparison of linear and nonlinear adaptive control of a ph-process. *IEEE Control Syst. Magazine* 28, 781–785.
- Pajunen, G.A. (1992). Adaptive control of Wiener type nonlinear systems. Automatica 28, 4, 781–785.
- Pearson, R.K. (2003). Selecting nonlinear model structures for computer control. J. of Process Control 13, 1–26.
- Pearson, R.K. and M. Pottmann (2000). Graybox identification of block-oriented nonlinear models. J. of Process Control 10, 301–315.
- Wahlberg, B. (1991). System identification using Laguerre models. *IEEE Transactions on Au*tomatic Control 36, 5, 551–562.
- Wahlberg, B. (1994). System identification using Kautz models. *IEEE Transactions on Auto*matic Control **39**, **6**, 1276–1282.
- Wigren, T. (1994). Recursive prediction error identification using the nonlinear Wiener model. Automatica 29, 4, 1011–1025.
- Wigren, T. (1999). Recursive Identification Based on The Nonlinear Wiener Model. Prentice-Hall Inc.. Englewood Cliffs, NJ.