Nonlinearity Quantification and its Application to Nonlinear System Identification

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ABSTRACT

In a series of previous works (Nikolaou, 1993) we introduced an inner product and a corresponding 2-norm for discrete-time nonlinear dynamic systems. Unlike induced norms of nonlinear systems, which are difficult to compute (albeit extremely useful), the 2-norm mentioned above is straightforward to compute, through Monte Carlo calculations with either experimental or simulated data. Loosely speaking, the 2-norm captures the average effect of a class of inputs on the output of a dynamic system. In this presentation we will give a brief introduction to this 2-norm, based on our previous results, and will discuss our latest work and applications on this subject. In particular, we will address the following points: (a) How is the nonlinearity of a dynamic system quantified by the 2-norm? (b) How adequate is a linear model for the representation of a nonlinear system? (c) What nonlinear model can be used for the representation of a nonlinear system for which a linear model is inadequate? An important result of this theory is that appropriate orthogonal bases for the representation of a nonlinear dynamic system can be constructed, that allow the successive refinement of a moving average nonlinear model through inclusion of additional basis terms, without requirement for readjustment of the entire model. Parallel (neural) implementation issues for the proposed algorithms are discussed. Nonlinear models based on Volterra-Legendre series are discussed in detail; and (d) How does feedback alter the nonlinearity characteristics of a dynamic system? Examples on four chemical processes are presented to elucidate the computational and conceptual merits of the proposed methodologies.

Introduction

The claim that most chemical processing systems have nonlinear dynamics is well documented in literature (Shinskey, pp. 55-56, 1967; Foss, 1973; Buckley, 1981; García and Prett, 1986; Morari, 1986; IEEE Report, 1987; NRC Committee Report, p. 148, 1988; Fleming, 1988; Prett and García, p. 18, 1988; Edgar, 1989; Longwell, 1991; Bequette, 1991; Kane, 1993; Doyle and Allgöwer, 1996; Ogunnaike and Wright, 1996). Nonlinear processes include exothermic and autocatalytic reactors, thermally coupled or high purity distillation towers, supercritical extractors, and refrigeration units. The modeling of nonlinear systems has attracted the interest of several researchers, particularly in view of using nonlinear dynamic models for nonlinear control. The explosion in the use of neural network models (triggered by the re-invention of back-propagation by Rumelhart *et al*. (1986)), research on model-predictive control for nonlinear systems (Muske and Rawlings, 1993; Genceli and Nikolaou, 1995; Mayne, 1996), and studies on exact-linearization methods (Isidori, 1989; Nijmeijer and van der Schaft, 1990; Kravaris and Kantor, 1990; Kumar and Daoutidis, 1996; Soroush and Kravaris, 1996) are only but a few areas where researchers have tried to tame nonlinearities. The extent to which process nonlinearities may be significant (for an explicitly stated task) is often assessed through experience and general rules of thumb. For instance, Arrhenius ($e^{-E/RT}$) type of nonlinearities are often classified as “severe”, while polynomial type of nonlinearities are classified as “mild”. It is clear that a more quantitative assessment of a dynamic system’s nonlinearity would be useful. To establish a nonlinearity quantifier, one should clearly state the purpose for which that quantifier is developed. For example, it is well known that there exist nonlinear reactors for which, due to nonlinearity, the sign of the steady state gain changes in different operating regimes, causing instability problems when the reactor is regulated by a linear feedback controller (Morari and Zafiriou, 1989). Clearly, from the viewpoint of linear feedback control, such reactors are severely nonlinear. A problem we address in this article is the quantification of nonlinearity for open and closed-loop systems. As stressed in review articles on nonlinear control (Bequette, 1991) and nonlinear model-predictive control (Rawlings et al., 1994), the issues of determining whether a nonlinear control strategy is needed for a particular process, and developing a nonlinear model, if one is indeed needed, are assuming central position and make clear the need for new theoretical and computational tools. This work is an attempt to provide such tools.

In our previous work (Nikolaou, 1993) we constructed a general nonlinearity quantifier, through an inner-product-based 2-norm for nonlinear systems. The 2-norm creates a unifying mathematical framework for nonlinear system modeling. For instance, within that framework, the nonlinearity of a dynamic system *P* is quantified as

$$\frac{q}{V_1}(C_{Af}-C_A)$$

where $\|\bullet\|$ is the 2-norm, and L_{opt} is the optimal linear approximation of the system P that minimizes $\|L-P\|$. In this work we explore the 2-norm framework for modeling nonlinear systems with Volterra series. We show how to modify Volterra series (by using multidimensional Legendre polynomials) so that the corresponding Volterra kernels can be identified sequentially and independently of one another. We also hint to other possible modeling alternatives that may result in identification methods for which parameters can be identified independently of one another. Based on our framework, we show that polynomial nonlinearities may be "severe", while Arrhenius nonlinearities may be "mild". In addition, we demonstrate how *linear* feedback can drastically alter the nonlinearity characteristics of a nonlinear system, a fact long claimed (Black 1934; 1977) but not well quantified. We want to emphasize that our ambitions in this article are far below the development of all-inclusive tools that could handle all systems that are not linear (hence, by default, nonlinear). Nonlinear systems can exhibit extremely rich patterns of behavior (e.g. bifurcation or chaos), which may by further enriched if feedback is used. The class of nonlinear systems that we study is precisely defined in the main text. It should be mentioned that there exists a significant body of literature dealing with the nonlinearity of systems without inputs, in a time-series framework (Tong, 1990; Tsay, 1991; Theiler et al., 1992).

The rest of the paper is structured as follows: A unifying framework is presented first for nonlinear system modeling, entailing a nonlinear system inner product and 2-norm and the concepts of orthogonality, projection and optimal approximation. Models based on orthogonal nonlinear operator bases are presented next, followed by a discussion on model-predictive control with Volterra-Legendre models. Case studies follow, and subsequently conclusions are drawn. Readers with a main interest in applications, may skip the theoretical developments and directly start with the case studies, from within which they can back track useful formulas developed in the main text.

A Unifying Framework for Nonlinear System Modeling

Basic background

We will first define the notion of nonlinear operator P, which is a mapping of an input sequence to an output sequence. Then we will show how to construct an inner product $\langle P;Q \rangle$ between two nonlinear operators P and Q, which will lead us to the 2-norm of P. The implications of the constructed inner-product space for nonlinear system modeling will then be elaborated on. For details and proofs of subsequent theorems see Nikolaou (1993).

Definition 1: An unbiased nonlinear operator P, corresponding to *nosteps* time-steps (with *nosteps* in $\mathbf{N} \cup \{\infty\}$), is defined as a continuous mapping from $\Re^{nosteps}$ to $\Re^{nosteps}$, such that the input sequence vector

$$\mathbf{u} \hat{=} [u_1, u_2, u_3, \ldots, u_{nosteps}]^T \tag{1}$$

is mapped to the output sequence

$$\mathbf{y} \hat{=} [y_1, y_2, \ldots, y_{nosteps}]^T = P\mathbf{u} \hat{=} [(P\,\mathbf{u})_1, (P\,\mathbf{u})_2, \ldots, (P\,\mathbf{u})_{nosteps}]^T \tag{2}$$

and

$$\mathbf{u} = \mathbf{0} \Rightarrow P\,\mathbf{u} = \mathbf{0} \tag{3}$$

Definition 2: The null operator, O, and the identity operator, I, are respectively defined as

$$O\,\mathbf{u} = \mathbf{0}, \text{ for all } \mathbf{u} \text{ in } \Re^{nosteps} \tag{4}$$

and

$$I\,\mathbf{u} = \mathbf{u}, \text{ for all } \mathbf{u} \text{ in } \Re^{nosteps} \tag{5}$$

Postulate: If $P \neq O$, then

$$P\,\mathbf{u} = \mathbf{0} \Leftrightarrow \mathbf{u} = \mathbf{0} \tag{6}$$

Remark 1: If the left inverse of P exists (i.e $P^{-1}P = I$), then

$$P\,\mathbf{u} = \mathbf{0} \Rightarrow P^{-1}P\,\mathbf{u} = P^{-1}\mathbf{0} \Rightarrow \mathbf{u} = \mathbf{0} \tag{7}$$

Therefore, the existence of the left inverse of an unbiased nonlinear operator implies the above equivalence (6).

Theorem 1 (Nikolaou, 1993a)**:** The equation

$$\langle P;Q \rangle \hat{=} \lim_{\substack{noinputs \to \infty \\ \mathbf{u}^r \neq 0}} \left(\frac{1}{noinputs} \sum_{r=1}^{noinputs} \frac{\langle P\mathbf{u}^r, Q\mathbf{u}^r \rangle}{nosteps} \right) \tag{8}$$

defines an inner product $\langle P;Q \rangle$ of the operators $P: \Re^{nosteps} \to \Re^{nosteps}$ and $Q: \Re^{nosteps} \to \Re^{nosteps}$, where $\mathbf{u}^r$ is a random vector in

$$U \hat{=} [u_{\min}, u_{\max}] \times [u_{\min}, u_{\max}] \times \ldots \times [u_{\min}, u_{\max}] \subseteq (\Re \cup \{\pm\infty\})^{nosteps}$$

with probability distribution

$$p(u_1^r)\, p(u_2^r) \,.\,.\, p(u_{nosteps}^r) > 0 \text{ on } U, \tag{9}$$

and $\langle P\mathbf{u}^r, Q\mathbf{u}^r \rangle$ is any inner product of the vectors $P\mathbf{u}^r$ and $Q\mathbf{u}^r$ in $\Re^{nosteps}$. The standard inner product of the vectors $P\mathbf{u}^r$ and $Q\mathbf{u}^r$ is defined as

$$\langle P\mathbf{u}^r, Q\mathbf{u}^r \rangle \hat{=} \sum_{i=1}^{nosteps} (P\mathbf{u}^r)_i (Q\mathbf{u}^r)_i \tag{10}$$

Remark 2: The probability distribution $p(u_1^r)\, p(u_2^r) \,.\,.\, p(u_{nosteps}^r)$ in inequality (9) can be either uniform on $[u_{\min}, u_{\max}]$, or any other continuous distribution that is nonzero everywhere on $[u_{\min}, u_{\max}]$. By selecting this distribution appropriately, the importance of various classes of input signals deviating from steady state at various levels can be quantified.

Remark 3: Although the standard inner product on $\Re^{nosteps}$ in eqn. (10) is used throughout this work, other inner products may be used. For example, inner products in Sobolev spaces (involving rates of change of the output signal) may be considered.

Remark 4: Theorem 1 suggests that for a given value of *nosteps*, $\langle P;Q \rangle$ can be computed through the following Monte Carlo calculations, either experimentally or through computer simulation if a model is available: Consider random inputs $\mathbf{u}^r$ in $\Re^{nosteps}$ with entries identically distributed in $[u_{\min}, u_{\max}]$, and compute the partial sums

$$S_{noinputs} \hat{=} \frac{1}{noinputs} \sum_{r=1}^{noinputs} \frac{\langle P\mathbf{u}^r, Q\mathbf{u}^r \rangle}{nosteps} \tag{11}$$

until the standard deviation

$$\sigma_{\langle P;Q\rangle} \hat{=} \sqrt{\sum_{r=1}^{noinputs} \frac{\left[\frac{\langle P\mathbf{u}^r, Q\mathbf{u}^r\rangle}{nosteps} - S_{noinputs}\right]^2}{noinputs(noinputs-1)}} \tag{12}$$

is small enough.

Definition 3: Let P: $\Re^{nosteps} \to \Re^{nosteps}$ be a continuous, discrete-time, nonlinear operator. Then the 2-norm of P is defined as

$$\|P\| \hat{=} \sqrt{\langle P;P\rangle} \tag{13}$$

Remark 5: If the induced norm of P over a set U is defined as

$$\|P\|_{ip} \hat{=} \sup_{\mathbf{u}\in U} \frac{\|P\mathbf{u}\|_p}{\|\mathbf{u}\|_p} \tag{14}$$

$$\overset{p=2}{\hat{=}} \sup_{\mathbf{u}\in U} \frac{\sqrt{\langle P\mathbf{u}, P\mathbf{u}\rangle}}{\sqrt{\langle \mathbf{u},\mathbf{u}\rangle}} \tag{15}$$

where U is a subset of an l_p space of p-summable sequences $\{u_i\}$ (i.e. such that $\left[\sum_i |u_i|^p\right]^{1/p} < \infty$, $1 \le p \le \infty$), and $\|.\|_p$ its corresponding norm over the set U (Nikolaou and Manousiouthakis, 1989), then

$$\|P\mathbf{u}\|_p \le \|P\|_{ip} \|\mathbf{u}\|_p \quad \text{for all } \mathbf{u}\in U \tag{16}$$

suggesting that $\|P\mathbf{u}\|_p$ is finite if P is stable and $\|\mathbf{u}\|_p$ is bounded. The above 2-norm derived through eqn. (13) is not induced, therefore it does not satisfy inequality (16). However, it is much easier to compute (Remark 3).

Nonlinear system modeling with the 2-norm

The problem of nonlinear system modeling is equivalent to optimally approximating a nonlinear operator *P* (corresponding to the real system) by another operator *A*, belonging to a certain class ***A*** of operators. This problem can be formulated (Desoer and Wang, 1975) as

$$\min_{A \in \boldsymbol{A}} \| A - P \| \tag{17}$$

where *A* is an operator belonging to a subspace ***A*** of operators over which the approximation is to be performed. Use of the 2-norm defined in eqn. (13) results in the well known fact that the optimal *A* is the orthogonal projection of *P* on ***A*** (Luenberger, 1969).

Finding an optimal linear approximation L *for a nonlinear system* P

In that case the subspace ***A*** contains linear operators of the form

$$L = \sum_{i=0}^{nopastu} h_i L_i \tag{18}$$

where L_i is a linear operator corresponding to a time-delay of *i* time steps, i.e.

$$L_i\, [u_1, u_2, u_3, \ldots, u_{nosteps}]^T = [u_{1-i}, \ldots, u_{-1}, u_0, u_1, u_2, u_3, \ldots, u_{nosteps-i}]^T =$$

$$= [\begin{array}{cccccccc} 0 & \cdots & 0 & u_1 & u_2 & \cdots & u_{nosteps-i} \\ \downarrow & \cdots & \downarrow & \downarrow & \downarrow & \cdots & \downarrow \\ 1 & \cdots & i & i+1 & i+2 & \cdots & nosteps \end{array}]^T \tag{19}$$

The optimal solution

$$L_{opt} = \sum_{i=0}^{nopastu} h_i L_i$$

of the minimization problem in (17) is given by the equation (Nikolaou, 1993)

$$\Phi\, \mathbf{h} = \chi \tag{20}$$

where

$$\Phi = \begin{bmatrix} \langle L_0; L_0 \rangle & \langle L_0; L_1 \rangle & \cdots & \langle L_0; L_{nopastu} \rangle \\ \langle L_1; L_0 \rangle & \langle L_1; L_1 \rangle & \cdots & \langle L_1; L_{nopastu} \rangle \\ \vdots & . & \ddots & \vdots \\ \langle L_{nopastu}; L_0 \rangle & \langle L_{nopastu}; L_1 \rangle & \cdots & \langle L_{nopastu}; L_{nopastu} \rangle \end{bmatrix}$$

$$\mathbf{h} = [h_0 \;\; h_1 \; \cdots \; h_{nopastu}]^T$$

$$\chi = \left[\langle L_0; P \rangle \;\; \langle L_1; P \rangle \;\; \cdots \;\; \langle L_{nopastu}; P \rangle \right]^T$$

and the inner product of two operators from the basis set $\{L_i\}_{i=0}^{nopastu}$ is (Nikolaou, 1993)

$$\langle L_i; L_j \rangle = \begin{cases} \dfrac{nosteps - \max(i, j)}{4nosteps}(u_{\max} + u_{\min})^2 & \text{if } i \neq j \\ \| L_i \|^2 = \dfrac{nosteps - i}{3nosteps}(u_{\max}{}^2 + u_{\max}u_{\min} + u_{\min}{}^2) & \text{if } i = j \end{cases} \tag{21}$$

Details for this problem, such as approximation with auto-regressive-moving-average models, and robustness of identification, are discussed in Nikolaou (1993).

A quantifier of dynamic system nonlinearity

The importance of the result in the previous section is that *the value of*

$$\frac{\| L_{opt} - P \|}{\| P \|} \tag{22}$$

quantifies the magnitude of the nonlinearity of the nonlinear dynamic system P. Since

$$\frac{\| L_{opt} - P \|}{\| P \|} \geq \frac{\left| \| L_{opt} \| - \| P \| \right|}{\| P \|}$$

the right-hand side of the above inequality is an obvious lower bound for the nonlinearity magnitude of a system. The importance of the above quantities will be illustrated in the case studies.

Finding an optimal nonlinear approximation N ***for a nonlinear system*** P

If the subspace ***A*** contains nonlinear operators N that correspond to a nonlinear moving-average type of model (i.e. $y_k = f(u_k, u_{k-1}, u_{k-2},..., u_{k-nopastu})$), then we have that

$$\mathbf{y} \hat{=} [y_1, y_2, \ldots, y_{nosteps}]^T =$$

$$= \left[f(u_1, u_0, ..., u_{1-nopastu}), \cdots, f(u_{nosteps}, u_{nosteps-1}, ..., u_{nosteps-nopastu})\right]^T$$

which implies that the form of the operator N depends on the form of the function $f\colon \Re^{nopastu+1} \to \Re$. Approximating a function f has been the subject of intensive research in recent years (Hopfield, 1982; Rumelhart et al., 1986; Friedman, 1991; Bakshi and Stephanopoulos, 1993). The approximation we will consider in this work relies on the standard representation of an element in a vector space as a linear combination of basis elements of that space, i.e.

$$f = \sum_{i=1}^{nobases} g_i f_i \tag{23}$$

where $\{f_i\colon \Re^{nopastu+1} \to \Re\}_{i=1}^{nobases}$ is the set of basis functions in the *nobases*-dimensional space of functions by which f will be approximated. Equation (23) implies that

$$N = \sum_{i=1}^{nobases} g_i N_i \tag{24}$$

where $N_i\colon \Re^{nosteps} \to \Re^{nosteps}$ is the nonlinear operator defined by

$$N_i\, [u_1, u_2, u_3, ..., u_{nosteps}]^T =$$

$$= \left[f_i(u_1, u_0, ..., u_{1-nopastu}), \cdots, f_i(u_{nosteps}, .., u_{nosteps-nopastu})\right]^T =$$

$$= \left[f_i(u_1, 0, ..., 0), \cdots, f_i(u_{nosteps}, ..., u_{nosteps-nopastu})\right]^T \tag{25}$$

Theorem 5 (Nikolaou, 1993a)**:** The solution

$$N_{opt} = \sum_{i=1}^{nobases} a_i N_i$$

of the problem

$$\min_N \|N - P\|$$

with N being a nonlinear operator represented by eqn. (24), is uniquely determined by the linear system of equations

$$\Psi \, \mathbf{a} = \xi \tag{26}$$

where

$$\Psi = \begin{bmatrix} \langle N_1; N_1 \rangle & \langle N_1; N_2 \rangle & \cdots & \langle N_1; N_{nobases} \rangle \\ \langle N_2; N_1 \rangle & \langle N_2; N_2 \rangle & \cdots & \langle N_2; N_{nobases} \rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle N_{nobases}; N_1 \rangle & \langle N_{nobases}; N_2 \rangle & \cdots & \langle N_{nobases}; N_{nobases} \rangle \end{bmatrix}$$

$$\mathbf{a} = [a_1 \;\; a_2 \;\; \ldots \;\; a_{nobases}]^T$$

$$\xi = [\langle N_1, P \rangle \;\; \langle N_2, P \rangle \;\; \cdots \;\; \langle N_{nobases}, P \rangle]^T$$

Theorem 6 (Nikolaou, 1993a)**:** If the functions $\{f_i: \Re^{nopastu+1} \to \Re\}_{i=1}^{nobases}$ of eqn. (24) are orthogonal to one another in the interval $[u_{\min}, u_{\max}]$, in the sense

$$\int_{u_{\min}}^{u_{\max}} \cdots \int_{u_{\min}}^{u_{\max}} f_i(x_0, \cdots, x_{nopastu}) f_j(x_0, \cdots, x_{nopastu}) dx_0 \cdots dx_{nopastu} = 0, \quad i \neq j \tag{27}$$

then

$$a_i = \frac{\langle N_i; P \rangle}{\langle N_i; N_i \rangle} = \frac{\langle N_i; P \rangle}{\| N_i \|^2}, \quad i = 1, \ldots, nobases < nosteps \tag{28}$$

Corollary 6: If the set of operators $\{N_i\}_{i=1}^{nobases}$ are orthogonal, then the coefficients $\{a_i\}_{i=1}^{nobases}$ satisfy *Bessel*'s inequality

$$\sum_{i=1}^{nobases} \| N_i \|^2 | a_i |^2 \leq \|P\|^2 \tag{29}$$

If $P = \sum_i^{nobases} a_i N_i$, then Bessel's inequality becomes Parseval's equality.

Remark 6: Theorem 6 shifts the orthogonality between the operators N_i and N_j to the orthogonality of the functions f_i and f_j. This allows a large number of possible options for the selection of $\{f_i\}_{i=1}^{nobases}$, including orthogonal polynomials (e.g. Legendre), Fourier bases, functions with compact support such as wavelets (Bakshi and Stephanopoulos, 1993) etc. The values of the coefficients a_i can be determined independently of one another. This greatly simplifies the approximation process, since additional terms $a_i N_i$ can be included in the sum of eqn. (24) until nonlinearity is adequately approximated. The potential for parallel (neural) computation is obvious, and is enhanced if the parallelism described in Remark 3 is considered.

Remark 7: Standard Gram-Schmidt orthonormalization of $\{N_i\}_{i=1}^{nobases}$ can yield a set of orthonormal bases $\{G_i\}_{i=1}^{nobases}$ as follows:

$$Y_1 = L_1, \qquad G_1 = Y_1/\|Y_1\|$$

$$Y_{i+1} = L_{i+1} - \sum_{j=1}^{i} \left\langle L_{i+1}; G_j \right\rangle G_j \ , \qquad G_{j+1} = Y_{j+1}/\|Y_{j+1}\|$$

Remark 8: For a nonlinear system

$$P = \sum_{i=1}^{nobases} a_i G_i$$

modelled by

$$P_m = \sum_{i=1}^{nobases} a_{m,i} G_i$$

with uncertainties $\delta a_i \mathrel{\hat{=}} a_i - a_{m,i}$ in the coefficients a_i, Parseval's equality, i.e.

$$\|\Delta P\|^2 = \sum_{i=0}^{nobases} \| G_i \|^2 | \delta a_i |^2 = \|\delta \mathbf{a}\|_2^2$$

indicates that $\|\delta \mathbf{a}\|_2^2 \mathrel{\hat{=}} \sum_{i=1}^{nobases} \delta a_i^2$ *is a measure of the overall modeling uncertainty* $\Delta P \mathrel{\hat{=}} P - P_m$. *A small error in the optimal coefficients* a_i *produces a small error in the approximation of* P.

Nonlinear models based on orthogonal basis operators

As stated above, a large number of candidate bases f_i may be considered for the construction of the basis operators N_i. Next we present a discussion on the use of polynomial (Volterra-type) series. Details of other nonlinear bases will be examined in forthcoming publications.

Approximation with polynomial model.

The use of Volterra series for nonlinear system modeling is discussed in detail in Schetzen (1980), Rugh (1983), Boyd and Chua (1985). For second-order discrete time Volterra series we have

$$y_k = f(u_k, \dots, u_{k\text{-}nopastu}) = \sum_{i=0}^{nopastu1} a_i u_{k-i} + \sum_{i=0}^{nopastu2} \sum_{j=0}^{nopastu2} b_{ij} u_{k-i} u_{k-j} \tag{30}$$

where

$$nopastu = \max\{nopastu1, nopastu2\}$$

The above equation shows that f is a second-degree multidimensional polynomial, expressed in terms of the polynomial basis functions

$$\{1, u_0, \dots, u_{nopastu}, u_0 u_1, \dots, u_0 u_{nopastu}, \dots, \dots u_{nopastu} u_{nopastu}\}. \tag{31}$$

The above set is not orthogonal in the symmetric interval $[-u_{\max}, u_{\max}]$. For example,

$$\int_{-u_{\max}}^{u_{\max}} \dots \int_{-u_{\max}}^{u_{\max}} u_i^2 u_j^2 du_0 du_1 \cdots du_{nopastu} = \frac{2^{nopastu+1}}{9} u_{\max}{}^{nopastu+7} \neq 0 \tag{32}$$

This does not allow the independent identification of the parameters $\{a_i\}$ and $\{b_{ij}\}$ (Pearson et al., 1992). A more convenient representation that utilizes orthogonal bases, stemming from Legendre polynomials, is as follows:

$$y_k = \sum_{i=0}^{nopastu1} \frac{\alpha_i}{u_{\max}} u_{k-i} + \sum_{i=0}^{nopastu2} \sum_{j=0}^{nopastu2} \beta_{ij} \left(\frac{3}{u_{\max}{}^2} u_{k-i} u_{k-j} - \delta_{ij} \right) + \sum_{i=0}^{nopastu2} \beta_{ii} \tag{33}$$

It is straightforward to show that the set of bases f_i considered in the above expression is orthogonal, hence resulting in orthogonal bases N_i. Its advantage is that the coefficients $\{\alpha_i\}$ and $\{\beta_{ij}\}$ can be identified independently of one another.

Remark 9: The above comment about the kernels being identifiable independently of one another can be extended to kernels of higher order. The importance of this fact is that in nonlinear system identification with orthogonal polynomial models the order of the polynomial (Volterra-Legendre) approximation and the number of past inputs included in the model can be increased in a *sequential* manner, without having to recalculate optimal values for the model coefficients. Thus, different numbers of past inputs (*nopastu*1, *nopastu*2) may be successively considered for the first- and second-order terms. In addition, terms of order 3, 4, $\cdots$ with small values for *nopastu*3, *nopastu*4, $\cdots$ may be successively introduced. This greatly simplifies the identification procedure and provides significant insight into the nature of the system modelled.

Approximation with multivariable harmonic model.

For basis functions f_j selected as

$$f_j(x_0, x_1, \ldots, x_{nopastu}) = \exp[\mathrm{i} \frac{\pi}{u_{\max}} \sum_{n=0}^{nopastu} k_{jn} x_n]$$

(where i is the imaginary unit) orthogonality in the interval $[-u_{\max}, u_{\max}]$ is straightforward to establish. Sequential identification can then be carried out in a standard way, as explained above.

Model-predictive control with Volterra-Legendre models

To use a Volterra-Legendre model or an equivalent standard Volterra model for model-predictive control, one can take at least two approaches:

Approach 1: Doyle et al. (1993) have shown how to use second-order Volterra models for the design of unconstrained model-predictive controllers. Their technique relies on the inversion of the nonlinear Volterra model, provided the inverse is stable. Zafiriou (1993) has examined the stability of the resulting closed loop.

Approach 2: A Volterra model can also be used in model-predictive control based on on-line optimization, particularly for problems with constraints. For constrained MPC with nonlinear models, most efforts have concentrated on numerical aspects of the on-line nonlinear optimization that MPC performs (Biegler and Rawlings, 1991; Gattu and Zafiriou, 1992; Sistu et al., 1993). In a recent development, Meadows and Rawlings (1993) use a state-space approach to derive stability conditions for constrained nonlinear MPC systems without modeling uncertainty, and show that unexpected difficulties may lurk behind seemingly well-behaved nonlinear systems. They demonstrate that through a nonlinear state-space system with polynomial nonlinearity, for which only discontinuous state feedback can result in closed-loop stability. Robust stability conditions for constrained MPC with Volterra models are developed in Genceli and Nikolaou (1994).

Since the emphasis of this work is on modeling rather than controller design, we will not discuss theoretical issues of either approach. We will use both approaches in the case studies that follow for illustration purposes.

Case studies

We will consider four reactor systems. For these systems we will assess open and closed-loop nonlinearities. In addition, we will show how Volterra-Legendre series can be developed for a system with significant nonlinearities.

Case study 1

Henson and Seborg (1990) studied the control of a two-continuous-stirred-tank-reactor-in-series system (2CSTR) modeled by the nonlinear differential equations

$$\frac{dC_{A1}}{dt} = \frac{q}{V_1}(C_{Af} - C_{A1}) - k_0\, C_{A1} \exp\left[-\frac{E}{RT_1}\right]$$

$$\frac{dT_1}{dt} = \frac{q}{V_1}(T_f - T_1) + \frac{(-\Delta H)k_0 C_{A1}}{\rho C_p} \exp\left[-\frac{E}{RT_1}\right] + \frac{\rho_c C_{pc}}{\rho C_p V_1} q_c \left(1 - \exp\left[\frac{hA_1}{q_c \rho_c C_{pc}}\right]\right)(T_{cf} - T_1)$$

$$\frac{dC_{A2}}{dt} = \frac{q}{V_2}(C_{A1} - C_{A2}) - k_0\, C_{A2} \exp\left[-\frac{E}{RT_2}\right]$$

$$\frac{dT_2}{dt} = \frac{q}{V_2}(T_1 - T_2) + \frac{(-\Delta H)k_0 C_{A2}}{\rho C_p} \exp\left[-\frac{E}{RT_2}\right] +$$

$$+ \frac{\rho_c C_{pc}}{\rho C_p V_2} q_c \left(1 - \exp\left[\frac{hA_2}{q_c \rho_c C_{pc}}\right]\right)\left(T_1 - T_2 + \exp\left[\frac{hA_1}{q_c \rho_c C_{pc}}\right](T_{cf} - T_1)\right).$$

An irreversible exothermic reaction,

$$A \xrightarrow{k} B$$

occurs in the two reactors. Notation and numerical values are provided in Table 1. Approximation of the derivatives in the model equations by forward finite differences ($\delta\tau$ = 0.1) defines the (discrete-time) nonlinear operator

$$P_{2CSTR}: \ [u_1, u_2, u_3, \ldots, u_{nosteps}]^T \to [y_1, y_2, \ldots, y_{nosteps}]^T$$

The linearization L_S of P_{2CSTR} around the steady state (u, y) = (0, 0), is realized by linear difference equations.

We apply our theory to examine the nonlinearity characteristics of the above system. The code was written in FORTRAN 77. The subroutine RNUN from the IMSL (1989) library was used for random number generation. All calculations were performed in a Sun SparcStation 1.

Application of equations (20) and (21) yielded the results of Figure 1. It can be seen that for inputs u in the ranges [– 0.01, 0.01], [– 0.05, 0.05] and [–0.10, 0.10] the coefficients h_i for the optimal linear approximations $L_{opt,j}$ are virtually identical to those of the linearization L_S of P_{2CSTR} around its steady state. This, however, does *not* suggest that the nonlinearity of the operator P_{2CSTR} is negligible for these ranges of inputs, as one might expect. This statement is supported by the results of Table 2, where the 2-norms of P_{2CSTR}, $L_{opt,1}$, … , $L_{opt,4}$, and L_S in growing intervals [$u_{\min}$, $u_{\max}$] are shown to be increasingly different. (Recall that $\|P - A\| \geq \big| \|P\| - \|A\| \big|$.) Table 3 shows the nonlinearity magnitude of P_{2CSTR}, and provides additional evidence of the severe nonlinearity of this system. Figures 2 to 4 compare step responses of the CSTR for inputs of magnitudes 0.01, 0.05, 0.10, to step responses of L_S and $L_{opt,j}$. There is significant discrepancy between P_{2CSTR} and L_S as well as between P_{2CSTR} and $L_{opt,j}$, as predicted by Tables 2 and 3. It should be mentioned that Henson and Seborg (1990) intuitively arrived at similar qualitative conclusions, by considering step response simulations.

Given the high nonlinearity of this system, we attempted to model it with second-order Volterra-Legendre series. The identification results are shown in Figures 5 to 8. In particular, *as many first and second order terms can be retained, as necessary. The retained nonzero terms will be optimal, and will not have to be readjusted after the deletion of essentially zero terms, or after the possible addition of third order terms*. Comparison between Figures 2 to 4 (step responses of the actual system and its linear approximations) and Figures 9 and 10 (step responses of the actual system and its second-order Volterra-Legendre approximations) shows that second-order Volterra-Legendre series can produce a significantly improved model of this system.

It should also be mentioned that no computational sophistication was used to accelerate the Monte-Carlo simulations or smoothen the results. It is conjectured that more accurate results can be obtained if these two actions are taken.

The next question that we pose for this reactor is "How are the nonlinearity characteristics of the reactor altered if a linear feedback controller is used?" To design the controller, we use the standard linear internal model control (IMC) methodology (Morari and Zafiriou, 1989), applied to the linear model L_s (linearization of P_{2CSTR} around the steady state)[2]. Several different values of α are used in the IMC filter

$$F(z) = \left(\frac{1-\alpha}{z-\alpha}\right)^2$$

The results (for inputs in the interval [–0.05, 0.05]) are shown in Table 4 and Figs. 11 and 12. Small α results in aggressive control action corresponding to large inputs *u* to the process. Such inputs drive the process to high nonlinearity regimes. On the other hand, large α results in "small" control action *u*, that makes the nonlinearity of the process less pronounced (Fig. 14). As Table 4 predicts, despite the fact that the open-loop system is "strongly" nonlinear (as demonstrated by the results in Tables 2 and 3), *the closed-loop system is significantly **less** nonlinear*. This is illustrated in Fig. 13, where closed-loop responses of the process with linear feedback control are compared to the ideal linear response F(z) that would result if the process were linear. The linearizing effects of feedback are clear. Such effects have long been claimed (Black, 1934; 1977) but hardly ever quantified. For verification purposes, Figs. 15 to 18 show simulations for the rejection of an external disturbance (T_f).

Case study 2

Nikolaou and Hanagandi (1993) studied a non-isothermal continuous stirred tank reactor (CSTR) modelled by the equations (Stephanopoulos, 1984)

$$\frac{dC_A}{dt} = \frac{F_I}{V}[C_{AI} - C_A] - k\, C_A \exp\left(-\frac{E}{RT}\right)$$

$$\frac{dT}{dt} = \frac{F_I}{V}[T_I - T] - \frac{\Delta H_R}{\rho C_P} k\, C_A \exp\left(-\frac{E}{RT}\right) - \frac{Q}{\rho C_P V}$$

---

[2] It should be noted that Henson and Seborg (1990) compared their nonlinear (exact-linearization based (Isidori, 1989; Kravaris and Kantor, 1990)) controller to a linear PI controller. That is not an entirely fair comparison, since a PI is not the best linear controller that can be used for that process. In fact, as shown by the results of Table 7, a linear IMC controller may be comparable to a nonlinear controller, as verified by the simulations in Fig. 7. This makes clear the importance of being able to *quantitatively* characterize nonlinearities.

Parameter values are shown in Table 5. This reactor has an Arrhenius type of nonlinearity, which is usually considered severe. As Tables 6 and 7 show, application of the 2-norm theory reveals that, *on the average*, this is *not* the case for inputs in the intervals [-0.10, 0.10], [-0.40, 0.40] and [-0.50, 0.50]. Table 8 shows the 2-norm for the closed-loop operator P_{CL} when a linear IMC controller with a first-order filter $\frac{1-\alpha}{z-\alpha}$ is used. The set-point y^{SP} varied in the range [±0.0547894] corresponding to a ±30 K change in temperature. Table 8 shows the closed-loop nonlinearity. It remains low. Nonlinearity does become important for larger inputs. In fact, there is a significant advantage in using nonlinear vs. linear control if the system if forced to operate in the severe nonlinearity range, as shown by Nikolaou and Hanagandi (1993) who used a nonlinear controller based on a recurrent neural network model.

Case study 3

We will briefly summarize our conclusions for this example, treated in detail in Nikolaou (1993a). The reaction

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

occurs in an isothermal continuous stirred-tank reactor (ICSTR), modelled by the dimensionless equations (Ray, 1981)

$$\frac{dx}{dt} = -x - Da_1\, x^2 + 1 + u$$

$$\frac{dz}{dt} = Da_1\, x^2 - z - Da_2\, z^{1/2}$$

Notation and numerical values are provided in Table 9. Notice the natural lower bound on the input ***u***. Although the nonlinearity of this reactor is polynomial, hence "mild", it becomes significant if large enough inputs are considered (Tables 10 and 11). The important information provided by the 2-norm is *how large* inputs must be considered before nonlinearity becomes significant (e.g. inputs in [–1, 5] or [–1, 10]) and how significant it becomes.

A closed-loop with this reactor is also examined. The reactor nonlinearity is augmented by the saturation nonlinearity acting on the input (Fig. 19). Figure 20 shows that for small set-point changes tight control is more linearizing, while for larger set-point change ranges looser control is more linearizing, since it activates the saturation nonlinearity less frequently.

Case study 4

Uppal et al. (1974) studied the following reactor (U-CSTR).

$$\frac{dx_1}{dt} = -x_1 + Da(1-x_1)\exp\left[\frac{x_2}{1+\frac{x_2}{\gamma}}\right]$$

$$\frac{dx_2}{dt} = -x_2 + B\,Da(1-x_1)\exp\left[\frac{x_2}{1+\frac{x_2}{\gamma}}\right] + \beta(y_c - x_2) + d$$

$$y = x_2$$

Parameter definitions and values are given in Table 12. This reactor exhibits interesting nonlinear behavior, and has been studied extensively. Piovoso et al. (1993) studied the application of three nonlinear control strategies for this system. Nonlinear controller synthesis via system identification by neural networks was reported in Jones et al. (1994). Hernández and Arkun (1992) investigated the control related properties of a back-propagation neural network model of this reactor. Limqueco and Kantor (1990) constructed a nonlinear observer for the reactor model, after transforming it to a linear system with nonlinear output injection, and designed a globally linearizing controller for this system. As reported by Limqueco and Kantor (1990), a disturbance of –5 K in the feed temperature will produce drastic changes in the reactor temperature (ignition/extinction behavior).

Here we apply the 2-norm theory to investigate the nonlinearity of this reactor. The results are presented in Table 13. Comparison of the values in columns 3 and 4 in Table 13, shows that the system is "fairly" linear in the corresponding input ranges. This fact is supported by the linear variation of the system "gain" $\frac{\| P_{UCSTR} \|}{u_{\max}}$ vs. $u_{\max}$ as indicated in column 5. Fig. 21 shows the closed-loop performance of a linear IMC controller designed on the basis of $L_{opt,2}$, for different set-point changes. At t=40.0 a disturbance of –5 K in the feed temperature is introduced to demonstrate a large drift in temperature and at t=80.0 the linear IMC controller is turned on to bring the temperature to the steady state of 1.1. Comparing the linear controller performance with that of the nonlinear controller (reported in Limqueco and Kantor (1990)) again demonstrates that, for the set-point changes intended, linear control is still a good option.

Discussion and conclusions

The 2-norm introduced in our earlier work provides a framework for dealing with the problem of quantifying nonlinearities for dynamic systems. In this work we presented some extensions of the original theory, and examined its implications for modeling nonlinear systems with Volterra series. Our conclusion is that nonlinearities can be usefully *quantified* by the 2-norm for various ranges of process inputs. A nonlinear system may or may not necessitate the use of a nonlinear model, depending, of course, on the task for which this model is developed. For some nonlinear systems a linear model may be a very good approximation, provided inputs to the system remain within a certain range. In addition, even if a linear model may be a poor approximation for a real system, a linear model may be effectively used in controller design which can directly rival nonlinear controller design. Given the significant effort required to design and maintain nonlinear controllers (Bequette, 1991) a quantitative analysis of the need for such an approach would be a worthwhile task to complete before nonlinear control is attempted. For the specific case of modeling with Volterra series we showed how the proposed theory can be used to construct orthogonal Volterra series (based on Legendre polynomials) which greatly simplify the modeling process through sequential identification of Volterra kernels of various orders, independently of one another. Four case studies were presented to illustrate the above issues.

The theory presented in this paper has the potential for several extensions and applications. An extended list is presented in Nikolaou (1993a).

Nomenclature

A	operator (either linear or nonlinear): $\Re^{nosteps} \to \Re^{nosteps}$
α	parameter of the linear filter $F(z) = \left(\frac{1-\alpha}{z-\alpha}\right)^2$
Γ_i	linear operator $\Re^{nosteps} \to \Re^{nosteps}$, used as orthonormal basis in the representation of L
g_i, a_i	coefficients used in the representation of the nonlinear operators N, N_{opt} in terms of N_i
h_i	coefficients used in the representation of a linear operator in terms of L_i
I	the identity operator
L	linear operator: $\Re^{nosteps} \to \Re^{nosteps}$
L_i	linear operator $\Re^{nosteps} \to \Re^{nosteps}$, used as basis in the representation of L
$L_{opt,j}$	Optimal linear approximation of a nonlinear operator in the interval No. j
l_p	the space of sequence with finite p-norm
N	nonlinear operator: $\Re^{nosteps} \to \Re^{nosteps}$
N_i	basis nonlinear operator $\Re^{nosteps} \to \Re^{nosteps}$, used in the representation of N
nobases	the number of basis operators used for the representation of a nonlinear operator
noinputs	the number of input sequences considered in the calculation of the inner product of two operators
nopastu	the number of past values of the input u considered in a moving-average type of model
nosteps	the number of time-steps considered in the calculation of the inner product of two operators
O	the null operator: $\Re^{nosteps} \to \Re^{nosteps}$
P	nonlinear operator: $\Re^{nosteps} \to \Re^{nosteps}$
Q	nonlinear operator: $\Re^{nosteps} \to \Re^{nosteps}$
$\mathbf{0}$	the zero vector in $\Re^{nosteps}$
$\Re$	the set of real numbers
$\Re^n$	the set of n-dimensional real vectors
σ	standard deviation
s	steady state

u input sequence to a nonlinear system, $\hat{=}\ [u_1, u_2, \ldots, u_{nosteps}]^T$

$u_{\max}$ upper bound for the entries of the input vector **u**

$u_{\min}$ lower bound for the entries of the input vector **u**

y output sequence of a nonlinear system, $\hat{=}\ [y_1, y_2, \ldots, y_{nosteps}]^{\mathrm{T}}$

$y_{\max}^{SP}$ upper bound of y^{SP}

y^{SP} set-point of y

$\| . \|$ the 2-norm of an operator

$\| . \|_{ip}$ the induced p-norm of an operator

$\| . \|_p$ the p-norm of a vector in $\Re^n$, defined as $\left(\sum_{i=1}^{n} | u_i |^p\right)^{1/p}$ if $1 \leq p < \infty$; $\max_{i=1,\cdots,n} | u_i |$, if $p = \infty$

f nonlinear function: $\Re^{nosteps} \rightarrow \Re$

f_i nonlinear function: $\Re^{nosteps} \rightarrow \Re$, used as a basis in the representation of f

$\langle P;Q \rangle$ inner product of the operators P, Q

$\langle x, y \rangle$ inner product of the vectors x, y

Acronyms

ARMA Auto regressive moving average

CL CSTR closed loop

CSTR Continuous stirred tank reactor

ICL ICSTR closed loop

ICSTR Isothermal CSTR

MA Moving average

MARS Multivariate adaptive regression splines

UCSTR CSTR studied by Uppal et al. (1974)

2CSTR System of two CSTRs studied by Henson and Seborg (1990)

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Table 1. Parameters of 2CSTR (Henson and Seborg, 1990)

VARIABLE	DEFINITION	VALUE
C_{A1}, C_{A2}	Concentrations of species A in CSTRs 1 and 2	state variables
T_1, T_2	Temperatures of CSTRs 1 and 2	state variables
C_{Af}	Feed concentration of species A	1 mol/L
T_f	Feed temperature	350 K
T_{cf}	Coolant feed temperature	350 K
q	Feed flowrate	100 L/min
E/R	Activation energy	1×10^4 K
$V_1 = V_2$	Volumes of CSTRs 1 and 2	100 L
k_0	Reaction rate constant	7.2×10^{10} min^{-1}
u	$= \frac{q_c - q_{cs}}{q_{cs}}$; dimensionless coolant flowrate	input variable; ≥ -1
y	$= \frac{C_{A1} - C_{A1s}}{C_{A1s}}$; dimensionless reactant concentration	output
$-\Delta H$	Heat of reaction	4.78×10^{10} j/mol
$h A_1 = h A_2$	(Heat transfer coefficient) $\times$ (Area)	1.67×10^5 j/min/K
$C_p = C_{pc}$	Specific heat	0.239 j/g/K
$\rho = \rho_c$	density	1000 g/L
C_{A1s}	Steady state concentration of species *A* in CSTR 1	0.088228 mol/L
C_{A2s}	Steady state concentration of species *A* in CSTR 2	0.0052926 mol/L
T_{1s}	Steady state temperature of CSTR 1	441.2193 K
T_{2s}	Steady state temperature of CSTR 2	449.5177 K
q_{cs}	Steady state coolant flowrate	100 l/min

Table 2. Norms of P_{2CSTR}, its steady-state linearization L_s, and optimal linear approximations $L_{opt,j}$ over various input intervals $[u_{min}, u_{max}]$

j	$u_{max,j} = -u_{min,j}$	$\|P_{2CSTR}\|^2$	$\|L_s\|^2$	$\|L_{opt,1}\|^2$	$\|L_{opt,2}\|^2$	$\|L_{opt,3}\|^2$	$\|L_{opt,4}\|^2$	$\frac{\|P_{2CSTR}\|^2}{u_{max}^2}$
1	0.01	***4.30 10^–9^***	$4.56\ 10^{-9}$	***$4.57\ 10^{-9}$***	$4.62\ 10^{-9}$	$4.80\ 10^{-9}$	$6.00\ 10^{-9}$	$4.30\ 10^{-9}$
2	0.05	***$1.09\ 10^{-7}$***	$1.14\ 10^{-7}$	$1.14\ 10^{-7}$	***$1.16\ 10^{-7}$***	$1.20\ 10^{-7}$	$1.50\ 10^{-7}$	$4.37\ 10^{-9}$
3	0.10	***$4.61\ 10^{-7}$***	$4.56\ 10^{-7}$	$4.57\ 10^{-7}$	$4.63\ 10^{-7}$	***$4.80\ 10^{-7}$***	$6.00\ 10^{-7}$	$4.61\ 10^{-9}$
4	0.20	***$2.43\ 10^{-6}$***	$1.83\ 10^{-6}$	$1.83\ 10^{-6}$	$1.85\ 10^{-6}$	$1.92\ 10^{-6}$	***$2.40\ 10^{-6}$***	$6.07\ 10^{-9}$

Table 3. Error made in the approximation of P_{2CSTR} by linear operators over various input intervals $[u_{\min}, u_{\max}]$ (entries in bold/italics refer to nonlinearity magnitude)

j	$\frac{\|\| L_s - P_{2CSTR} \|\|}{\|\| P_{2CSTR} \|\|}$	$\frac{\|\| L_{opt,1} - P_{2CSTR} \|\|}{\|\| P_{2CSTR} \|\|}$	$\frac{\|\| L_{opt,2} - P_{2CSTR} \|\|}{\|\| P_{2CSTR} \|\|}$	$\frac{\|\| L_{opt,3} - P_{2CSTR} \|\|}{\|\| P_{2CSTR} \|\|}$	$\frac{\|\| L_{opt,4} - P_{2CSTR} \|\|}{\|\| P_{2CSTR} \|\|}$
1	0.34	***0.34***	0.34	0.33	0.36
2	0.37	0.37	***0.36***	0.36	0.38
3	0.46	0.44	0.44	***0.43***	0.44
4	0.77	0.77	0.76	0.75	***0.72***

Table 4. Assessment of closed-loop nonlinearity for 2CSTR

α	$\|\|P_{CL}\|\|^2$	$\|\|L_{opt}\|\|^2$	$\frac{\|\| L_{opt} - P_{CL} \|\|}{\|\| P_{CL} \|\|}$
0.4	2.73 10^{-7}	3.26 10^{-7}	***0.19***
0.5	2.15 10^{-7}	2.14 10^{-7}	***0.097***
0.6	1.60 10^{-7}	1.61 10^{-7}	***0.090***
0.7	1.14 10^{-7}	1.14 10^{-7}	***0.078***
0.9	3.24 10^{-8}	3.33 10^{-7}	***0.059***

Table 5. Parameters for CSTR (Nikolaou and Hanagandi, 1993)

VARIABLE	DEFINITION	VALUE
C_A	Concentration of species A	state variable
T	Temperature of the reactor contents	state variable
u	Dimensionless heat removal rate (= $\frac{Q-Q_s}{Q_s}$)	input
y	Dimensionless temperature (= $\frac{T-T_s}{T_s}$)	output
F_I	Inlet flowrate	1.133 m^3/hr
V	Reactor volume	1.36 m^3
C_{AI}	Inlet concentration of species A	8008.00 mol/m^3
k	Reaction constant	1.08×10^7 1/hr
E/R	Activation energy	8375.00 ˚K
ΔH_R	Heat of reaction	–69775.0 j/mol
T_I	Inlet feed temperature	373.3 ˚K
ρ	Density of reactor contents	800.80 kg/m^3
C_p	Specific heat	3140.00 J/(kg ˚K)
C_{As}	Steady state concentration of species A	393.300 mol/l
T_s	Steady state temperature	547.556 ˚K
Q_s	Steady state heat removal rate	1.066×10^8

Table 6. Norms of P_{CSTR}, its steady-state linearization L_s, and optimal linear approximations $L_{opt,j}$ over various input intervals $[u_{\min}, u_{\max}]$

j	$[u_{\min j}, u_{\max j}]$	$\|P_{ICSTR}\|^2$	$\|L_s\|^2$	$\|L_{opt,1}\|^2$	$\|L_{opt,2}\|^2$	$\|L_{opt,3}\|^2$	$\frac{\|P_{CSTR}\|}{u_{\max}}$
1	[-0.1, 0.1]	0.367	0.367	0.363	0.365	0.366	6.05
2	[-0.4, 0.4]	5.89	5.87	5.81	5.84	5.85	6.06
3	[-0.5, 0.5]	9.22	9.17	9.09	9.12	9.14	6.07

Table 7. Error made in the approximation of P_{CSTR} by linear operators over various input intervals $[u_{\min}, u_{\max}]$ (entries in bold/italics refer to nonlinearity magnitude)

j	$[u_{\min j}, u_{\max j}]$	$\frac{\| L_s - P_{CSTR} \|}{\| P_{CSTR} \|}$	$\frac{\| L_{opt,1} - P_{CSTR} \|}{\| P_{CSTR} \|}$	$\frac{\| L_{opt,2} - P_{CSTR} \|}{\| P_{CSTR} \|}$	$\frac{\| L_{opt,3} - P_{CSTR} \|}{\| P_{CSTR} \|}$
1	[-0.1, 0.1]	0.0167	***0.0174***	0.0170	0.0169
2	[-0.4, 0.4]	0.0231	0.0241	***0.0237***	0.0236
3	[-0.5, 0.5]	0.0291	0.0301	0.0297	***0.0295***

Table 8. Assessment of closed-loop nonlinearity for CSTR

α	$\|\|P_{CL}\|\|^2$	$\|\|L_{opt}\|\|^2$	$\frac{\|\| L_{opt} - P_{CL} \|\|}{\|\| P_{CL} \|\|}$
0.00	268	268	***0.0515***
0.50	100	101	***0.0463***
0.80	35.0	34.9	***0.0365***
0.90	16.6	16.5	***0.0301***
0.95	7.91	7.90	***0.00635***

Table 9. Parameters of ICSTR

VARIABLE	DEFINITION	VALUE
C_A, C_B	Concentrations of species *A* and *B* in the ICSTR	
C_{Af}, C_{Bf}	Concentrations of species *A* and *B* in the feed	
C_{Aref}	Reference concentration of species *A*	
F	Feed/effluent flowrate	
V	Reaction volume	
k_1, k_2	Reaction rate constants	
u	system input; (= $\frac{C_{Af}}{C_{Aref}}$)	≥ -1.0
x, z	system states (= $\left(\frac{C_A}{C_{Aref}}, \frac{C_B}{C_{Aref}}\right)$)	
y	Output (= (z - z_s))	
τ	dimensionless time (= $\frac{tF}{V}$)	
Da_1, Da_2	Damköhler numbers (= $\left(\frac{k_1 C_{Aref} V}{F}, \frac{k_2 V}{F C_{Aref}^{1/2}}\right)$)	(1.0, 2.0)
u_s	Steady state value of the input u	0.0
x_s, z_s	Steady state values of the states x, z	(0.61803399, 0.030825002)

Table 10. Norms of P_{ICSTR}, its steady-state linearization L_S, and optimal linear approximations $L_{opt,j}$ over various input intervals $[u_{\min}, u_{\max}]$

j	$[u_{\min j}, u_{\max j}]$	$\|\|P_{ICSTR}\|\|^2$	$\|\|L_S\|\|^2$	$\|\|L_{opt,1}\|\|^2$	$\|\|L_{opt,2}\|\|^2$	$\|\|L_{opt,3}\|\|^2$	$\|\|L_{opt,4}\|\|^2$
1	[– 0.1, 0.1]	***2.35 10^{-6}***	2.33 10^{-6}	***2.33 10^{-6}***	2.30 10^{-6}	1.48 10^{-5}	2.74 10^{-5}
2	[– 1, 1]	***2.35 10^{-4}***	2.33 10^{-4}	2.33 10^{-4}	***2.30 10^{-4}***	1.48 10^{-3}	2.74 10^{-3}
3	[– 1, 5]	***0.163***	2.67 10^{-2}	2.67 10^{-2}	2.67 10^{-2}	***0.166***	0.334
4	[– 1, 10]	***1.68***	0.132	0.132	0.132	0.820	***1.65***

Table 11. Error made in the approximation of P_{ICSTR} by linear operators $L_{opt,j}$ over various input intervals $[u_{min}, u_{max}]$ (entries in bold/italics refer to nonlinearity magnitude)

j	$\frac{\\| L_s - P_{ICSTR} \\|}{\\| P_{ICSTR} \\|}$	$\frac{\\| L_{opt,1} - P_{ICSTR} \\|}{\\| P_{ICSTR} \\|}$	$\frac{\\| L_{opt,2} - P_{ICSTR} \\|}{\\| P_{ICSTR} \\|}$	$\frac{\\| L_{opt,3} - P_{ICSTR} \\|}{\\| P_{ICSTR} \\|}$	$\frac{\\| L_{opt,4} - P_{ICSTR} \\|}{\\| P_{ICSTR} \\|}$
3	0.60	0.60	0.60	***0.16***	0.48
4	0.72	0.72	0.72	0.31	***0.13***

Table 12. Parameter values for UCSTR (Uppal et al., 1974)

VARIABLE	DEFINITION	VALUE
x_1	Dimensionless concentration of species *A*	state variable
x_2	Dimensionless temperature	state variable
γ	Dimensionless activation energy	20.0
β	Dimensionless heat transfer coefficient	0.3
B	Dimensionless adiabatic temperature rise	8.0
Da	Damköhler number	0.072
y_c	Dimensionless cooling jacket temperature	manipulated input
$y = x_2$		controlled output
d	Dimensionless feed temperature (disturbance)	0.0 (nominal value)
x_{1s}	Steady state values of the state x_1	0.1539693
x_{2s}	Steady state values of the state x_2	0.8859648
y_{cs}	Steady state value of the input	0.0

Table 13. Nonlinearity characteristics of P_{UCSTR} over various input intervals $[u_{\min}, u_{\max}]$

(entries in bold/italics refer to nonlinearity magnitude)

j	$[u_{\min j}, u_{\max j}]$	$\|P_{UCSTR}\|^2$	$\|L_{opt}\|^2$	$\frac{\| P_{UCSTR} \|}{u_{\max}}$	$\frac{\| P_{UCSTR} - L_{opt,2} \|}{\| P_{UCSTR} \|}$
1	[–1.0, 1.0]	$4.18\ 10^{-3}$	$4.24\ 10^{-3}$	0.0647	0.061
2	[–2.0, 2.0]	$1.74\ 10^{-2}$	$1.69\ 10^{-2}$	0.0329	***0.12***
3	[–2.5, 2.5]	$2.81\ 10^{-2}$	$2.65\ 10^{-2}$	0.0268	0.16