# A Model-Based Characterization of the Long-Term Asymptotic Behavior of Nonlinear Discrete-Time Processes Using Map Invariance 

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Index Terms-Nonlinear dynamical systems, discrete-time systems, map invariance, invariant manifolds, functional equations
Abstract-The present research work proposes a new approach to the problem of quantitatively characterizing the longterm dynamic behavior of nonlinear discrete-time processes. The formulation of the problem of interest can be naturally realized through a system of nonlinear functional equations (NFEs), for which a rather general set of conditions for the existence and uniqueness of a locally analytic solution is derived. The solution to the system of NFEs is then proven to represent a locally analytic invariant manifold for the nonlinear discretetime process of interest. The local analyticity property of the invariant manifold map enables the development of a series solution method for the above system of NFEs, which can be easily implemented using MAPLE. Under a certain set of conditions, it is shown that the invariant manifold attracts all system trajectories, and therefore, the long-term dynamic behavior is determined through the restriction of the discretetime process dynamics on the invariant manifold.

## I. Introduction

Most processes exhibit nonlinear behavior and are typically modeled by systems of nonlinear ordinary (ODEs) or partial differential equations (PDEs) in the continuoustime domain, or systems of nonlinear difference equations (DEs) in the discrete-time domain [2]. Despite the fact that the analysis of the dynamic behavior of linear processes can be performed with rigor and in a thorough manner, it still remains a rather challenging task for nonlinear processes [15]. Among the most notable research objectives in nonlinear process dynamic analysis is certainly the existence of invariant manifolds and the associated problem of finding/computing them. Notice, that the problem under consideration has been historically motivated by efforts to develop systematic methods for the simplification of the analysis of the behavior of nonlinear dynamical systems by effectively reducing the dimensionality of the original problem $[3,6,8,10,12,14]$. Within the above framework, the restriction of the system dynamics on the invariant manifold results in a lower-order dynamic model, and therefore, the latter essentially determines the system's long-term asymptotic behavior, since the original transition or approach to the manifold can be proven to be a rather fast one under certain conditions [15]. Furthermore, the study of invariant

[^0]manifolds has been primarily conducted in connection with the existence problem of (un)stable and center manifolds, stability, as well as bifurcation analysis [15]. However, it should be pointed out, that the classical stable and center manifold theory presupposes the successful transformation of the original nonlinear dynamical system into one whose Jacobian matrix of the linearized system around the equilibrium point of interest is in Jordan canonical form, and the corresponding stable, unstable and center eigenmodes appear as decoupled (the state space of interest being the direct sum of the stable, unstable and center eigenspaces) [15]. The latter requirement, while always achievable through a coordinate transformation, may result in a computationally demanding numerical problem particularly for higherorder systems, such as the ones obtained from discretization or modal decomposition tehnniques applied to distributed parameter systems [2]. Moreover, a conceptually similar geometric notion of a positively invariant finite-dimensional manifold was introduced in the study of the dynamic model reduction problem for parabolic PDE systems [2]. Finally, research results on symmetry-induced generalized invariants for distributed parameter systems were reported in [11].

The present research work proposes a new approach to the problem of quantitatively characterizing the long-term dynamic behavior of nonlinear discrete-time processes. The formulation of the problem of interest is realized through a system of nonlinear functional equations (NFEs), for which a rather general set of conditions for solvability is derived. In particular, the aforementioned set of conditions guarantees the existence and uniqueness of a locally analytic solution, which is then proven to be a locally analytic invariant manifold map for the nonlinear discrete-time process considered. It should be pointed out, that within the proposed framework of analysis, the formulation of the problem of interest does not presuppose the special structure of the Jacobian eigenspace of the linearized system required in the classical stable and center manifold theory, thus effectively overcoming the associated problems of computing the requisite transformation into the Jordan canonical form with the explicit decoupling of the stable, unstable and center eigenspaces, as well as the numerical solution to the associated eigenstructure problem [15]. Furthermore, the local analyticity property of the invariant manifold map enables the development of a series solution method that can be easily implemented using MAPLE. Under a certain set of conditions, it can be shown that the invariant manifold attracts all system trajectories, and therefore, the long-term dynamic behavior is calculated
through the restriction of the discrete-time process dynamics on the above invariant manifold.

## II. Mathematical Preliminaries

Nonlinear discrete-time dynamic processes are considered:

$$
\begin{equation*}
x(k+1)=F(x(k), w(k)) \tag{1}
\end{equation*}
$$

which are driven by the states of an exogeneous nonlinear discrete-time autonomous dynamical system:

$$
\begin{equation*}
w(k+1)=G(w(k)) \tag{2}
\end{equation*}
$$

where $k \in \mathcal{N}$ is the discrete-time index and $\mathcal{N}$ the set of positive integers, $x \in U^{n} \subset R^{n}$ is the process state vector, $w \in U^{m} \subset R^{m}$ is the state vector associated with dynamics (2), and $U^{n}, U^{m}$ are open subsets of the Euclidean spaces $R^{n}$ and $R^{m}$ respectively. Notice that the above dynamic process description may represent a process whose dynamics (1) is driven by:
(i) the input/disturbance dynamics (2), where input or disturbance changes are modelled as outputs of the exogeneous system (2), or
(ii) a time-varying process parameter vector $w(k)$ that follows dynamics (2) and models phenomena such as catalyst deactivation, enzymatic thermal deactivation, heat-transfer coefficient changes, etc., or
(iii) an upstream process modelled by (2), in which case, a cascade connection of the two nonlinear processes results in the "block-triangular" structure (1)-(2). It is assumed that the discrete-time process model (1)-(2) is obtained either through the employment of efficient discretization methods for the original continuous-time process, or through direct identification methods. It is also assumed that the $F(x, w)$ and $G(w)$ maps of the discrete-time dynamics (1)-(2) are real analytic vector functions defined on $U^{n} \times U^{m}$ and $U^{m}$ respectively. Without loss of generality, let the origin $x^{0}=0$ be an equilibrium point of (1): $F(0,0)=0$, that corresponds to $w^{0}=0$ with $G(0)=0$. The following assumption is also made:

Assumption 1: Matrix $A=\frac{\partial G}{\partial w}(0)$ has non-zero eigenvalues $k_{i},(i=1, \ldots, m)$ that all lie inside or outside the unit disc (Poincaré domain [15]). This assumption implies that the $w$ dynamics is either locally asymptotically stable or unstable, and that the $G(w)$ map is locally invertible around $w^{0}=0$.

The original nonlinear discrete-time dynamic process model (1)-(2) can be rewritten as follows:

$$
\begin{align*}
x(k+1) & =B x(k)+C w(k)+f(x(k), w(k)) \\
w(k+1) & =A w(k)+g(w(k)) \tag{3}
\end{align*}
$$

where $B, C$ are constant matrices with appropriate dimensions, and $f(x, w), g(w)$ are real analytic functions of $x$ and $w$ with $f(0,0)=g(0)=0$, and $\frac{\partial f}{\partial x}(0,0)=\frac{\partial f}{\partial w}(0,0)=$ $\frac{\partial g}{\partial w}(0)=0$.

The following definition is essential for the ensuing theoretical developments.

Definition 1 [15]: A set $S \subset R^{m+n}$ is said to be invariant under the nonlinear discrete-time dynamics (3) if for each $\left(x_{0}, w_{0}\right) \in S$, the orbit $\Omega=\{(x(k), w(k)), k \in \mathcal{N}\}$ of (3) satisfying $(x(k=0), w(k=0))=\left(x_{0}, w_{0}\right)$, is such that $(x(k), w(k)) \in S$ for all $k \in \mathcal{N}$. An invariant set $S \subset$ $R^{m+n}$ passing through the origin $\left(x^{0}, w^{0}\right)=(0,0)$ is said to be an analytic local invariant manifold of (3), if $S$ has the local topological structure of an analytic manifold around the origin.

## III. Main Results

Together with system (3) an associated system of nonlinear functional equations (NFEs) is also considered:

$$
\begin{align*}
\pi(A w+g(w)) & =B \pi(w)+C w+f(\pi(w), w) \\
\pi(0) & =0 \tag{4}
\end{align*}
$$

where $\pi: R^{m} \longrightarrow R^{n}$ is the unknown vector function of (4).

The following technical lemma reported in [9] is necessary.
Lemma 1 Let Assumption 1 hold true for system (1)(2). Consider the system of NFEs (4) and assume that the eigenvalues $k_{i},(i=1, \ldots, m)$ of matrix $A=\frac{\partial G}{\partial w}(0)$ are not related to the eigenvalues $\lambda_{j},(j=1, \ldots, n)$ of matrix $B=\frac{\partial F}{\partial x}(0,0)$ through any equations of the following type:

$$
\begin{equation*}
\prod_{i=1}^{m} k_{i}^{d_{i}}=\lambda_{j} \tag{5}
\end{equation*}
$$

( $j=1, \ldots, n$ ), where all the $d_{i}$ 's are non-negative integers with: $\sum_{i=1}^{m} d_{i}>0$. Then, the system of NFEs (4) admits a unique locally analytic solution $\pi(w)$ in a neighborhood of $w=0$.

Remark 1: Let us now consider the linear case where $G(w)=A w$ and $F(x, w)=B x+C w$, with $A, B, C$ being constant matrices with appropriate dimensions. Then, the unique solution to the system of functional equations (4) is given by: $\pi=\Pi w$, where $\Pi$ is the solution of the LyapunovSylvester matrix equation:

$$
\begin{equation*}
\Pi A-B \Pi=C \tag{6}
\end{equation*}
$$

It is known that the above linear matrix equation (6) admits a unique solution $\Pi$ as long as the eigenspectra of matrices $A, B$ are disjoined [7]. Notice, that the latter is guaranteed by the assumptions of Lemma 1, and therefore, the linear result is reproduced.

We are now in a position to present the paper's main results.

Theorem 1 Suppose that for system (1)-(2) Assumption 1 holds true, as well as the assumptions of Lemma 1. Then, there exists a neighborhood $V \subset R^{m}$ of $w^{0}=0$, and a
unique and locally analytic mapping $\pi: V \longrightarrow R^{n}$ such that:

$$
\begin{equation*}
S=\left\{(x, w) \in R^{n} \times V: x=\pi(w), \pi(0)=0\right\} \tag{7}
\end{equation*}
$$

is an analytic local invariant manifold of (1)-(2) (in the sense of Definition 1) that passes through the equilibrium point $\left(x^{0}, w^{0}\right)=(0,0)$, where $\pi(w)$ is the unique solution of the associated system of NFEs (4).

Proof: For the graph of the mapping $x=\pi(w)$ to be a local invariant manifold that passes through the origin $\left(x^{0}, w^{0}\right)=(0,0)$, it has to satisfy the following system of invariance NFEs:

$$
\begin{align*}
\pi(A w+g(w)) & =B \pi(w)+C w+f(\pi(w), w) \\
\pi(0) & =0 \tag{8}
\end{align*}
$$

The above condition can be easily deduced by applying the one-step forward in time operator on $x=\pi(w)$ and along an arbitrary solution curve $(x(k), w(k))$ of (1)-(2) which belongs to the manifold of interest, i.e. identically satisfies $x(k)=\pi(w(k))$. The above system of invariance NFEs (8) is exactly the system of NFEs (4) associated with the original discrete-time dynamics and the maps $F(x, w), G(w)$. Under the assumptions stated, the above system of NFEs (8) admits a unique and locally analytic solution in a neighborhood $V \subset R^{m}$ of $w^{0}=0$ due to Lemma 1. Therefore, the set (7) represents an analytic local invariant manifold of (1)-(2).

Remark 2: For practical reasons one must provide a solution scheme for the system of invariance NFEs (4). Notice, that $F(x, w), G(w), \pi(w)$ are locally analytic, and therefore, the proposed method suggests their expansion in Taylor series, followed by a procedure that equates the same order Taylor coefficients of both sides of (4). This procedure leads to recursion formulas, through which one can calculate the $N$-th order Taylor coefficients of the unknown solution $x=\pi(w)$, given the Taylor coefficients of $x=\pi(w)$ up to the order $N-1$ by solving a system of linear algebraic equations. In the derivation of the recursion formulas, it is convenient to use the following tensorial notation:
a) The entries of a constant matrix $A$ are represented as $a_{i}^{j}$, where the subscript $i$ refers to the corresponding row and the superscript $j$ to the corresponding column of the matrix.
b) The partial derivatives of the $\mu$-th component $F_{\mu}(x, w)$ of the vector function $F(x, w)$ with respect to the state variables $x$ evaluated at $(x, w)=(0,0)$ are denoted as follows: $F_{\mu}^{i}=\frac{\partial F_{\mu}}{\partial x_{i}}(0,0), F_{\mu}^{i j}=\frac{\partial^{2} F_{\mu}}{\partial x_{i} \partial x_{j}}(0,0), F_{\mu}^{i j k}=$ $\frac{\partial^{3} F_{\mu}}{\partial x_{i} \partial x_{j} \partial x_{k}}(0,0)$ etc., where $i, j, k, . .=1, \ldots, n$
c) The partial derivatives of the $\mu$-th component $F_{\mu}(x, w)$ of the vector function $F(x, w)$ with respect to the variables $w$ evaluated at $(x, w)=(0,0)$ are denoted as follows: $\bar{F}_{\mu}^{i}=$ $\frac{\partial^{i} F_{\mu}}{\partial w^{i}}(0,0)$, etc.
d) The standard summation convention where repeated upper and lower tensorial indices are summed up.

Under the above notation the $l$-th component $\pi_{l}(w)$ of the unknown solution $\pi(w)$ can be expanded in a multivariate Taylor series as follows:

$$
\begin{align*}
\pi_{l}(w) & =\frac{1}{1!} \pi_{l}^{i_{1}} w_{i_{1}}+\frac{1}{2!} \pi_{l}^{i_{1} i_{2}} w_{i_{1}} w_{i_{2}}+\ldots+ \\
& +\frac{1}{N!} \pi_{l}^{i_{1} i_{2} \ldots i_{N}} w_{i_{1}} w_{i_{2}} \ldots w_{i_{N}}+\ldots \tag{9}
\end{align*}
$$

and similarly for $F(x, w), G(w)$. Inserting the Taylor expansions of $\pi(w), F(x, w), G(w)$ into (4) and matching the Taylor coefficients of the same order, the following relation for the $N$-th order terms can be obtained:

$$
\begin{align*}
& \sum_{L=1}^{N} \sum_{0 \leq m_{1} \leq m_{2} \leq \ldots \leq m_{L}} \pi_{l}^{j_{1} \ldots j_{L}} G_{j_{1}}^{m_{1}} \ldots G_{j_{L}}^{m_{L}}=F_{l}^{\mu} \pi_{\mu}^{i_{1} \ldots i_{N}} \\
+ & \bar{F}_{l}^{i_{1} \ldots i_{N}}+f_{l}^{i_{1} \ldots i_{N}}\left(\pi^{i_{1} \ldots i_{N-1}}\right) \tag{10}
\end{align*}
$$

where $i_{1}, \ldots, i_{N}=1, \ldots, m, l=1, \ldots, n, \sum_{j=1}^{L} m_{j}=N$ and $f_{l}^{i_{1} \ldots i_{N}}\left(\pi^{i_{1} \ldots i_{N-1}}\right)$ is a function of Taylor coefficients of the unknown solution $\pi(w)$ calculated in the previous recursive steps. Note that the second summation symbol in (10) suggests summing up the relevant quantities over the $\frac{N!}{m_{1}!\ldots m_{L}!}$ possible combinations to assign the $N$ indices $\left(i_{1}, \ldots, i_{N}\right)$ as upper indices to the $L$ positions $G_{j_{1}} \ldots G_{j_{L}}$, with $m_{1}$ of them being put in the first position, $m_{2}$ of them in the second position, etc. $\left(\sum_{j=1}^{L} m_{j}=N\right)$. Furthermore, notice that equations (10) represent a set of linear algebraic equations in the unknown coefficients $\pi_{\mu}^{i_{1}, \ldots, i_{N}}$. Finally, a simple MAPLE code has been developed to automatically compute the Taylor coefficients of the unknown solution $x=\pi(w)$ of NFEs (4).

Theorem 2 Let matrix $B$ have stable eigenvalues $\left(\left|\lambda_{i}\right|<\right.$ $1, i=1, \ldots, n)$ and all assumptions of Theorem 1 hold true. Furthermore, let $S$ (7) be an invariant manifold of (1)-(2), where $\pi(w)$ is the solution to the associated system of invariance NFEs (4) and $(x(k), w(k))$ a solution curve of (1)-(2). There exists a neighborhood $U^{0}$ of the origin $\left(x^{0}, w^{0}\right)=(0,0)$ and a real number $M \in(0,1)$ such that, if $(x(0), w(0)) \in U^{0}$, then:

$$
\begin{equation*}
\|x(k)-\pi(w(k))\|_{2} \leq(M)^{k}\|x(0)-\pi(w(0))\|_{2} \tag{11}
\end{equation*}
$$

Proof: Denote by $z$ the "off-manifold" coordinate:

$$
\begin{equation*}
z(k)=x(k)-\pi(w(k)) \tag{12}
\end{equation*}
$$

whose dynamics is described by:

$$
\begin{align*}
& z(k+1)=B(z(k)+\pi(w(k)))+C w(k)+ \\
+ & f(z(k)+\pi(w(k)), w(k))- \\
- & B \pi(w(k))-C w(k)-f(\pi(w(k)), w(k))= \\
= & B z(k)+N(z(k), w(k)) \tag{13}
\end{align*}
$$

where: $N(z, w)=f(z+\pi(w), w)-f(\pi(w), w)$. Notice that $N(z, w)$ is a real analytic vector function with: $N(0,0)=$

0 and no linear terms in $z: \frac{\partial N}{\partial z}(0,0)=0$. Consequently: $\frac{\|N(z, w)\|_{2}}{\|z\|_{2}} \longrightarrow 0$ as $\|z\|_{2} \longrightarrow 0$, and thus, for an arbitrary constant $L>0$ there exist positive $\rho_{1}, \rho_{2}$, such that in the domain: $\|z\|_{2}<\rho_{1},\|w\|_{2}<\rho_{2}$ the following inequality holds:

$$
\begin{equation*}
\|N(z, w)\|_{2}<L\|z\|_{2} \tag{14}
\end{equation*}
$$

Furthermore, since matrix $B$ has all its eigenvalues with modulus less than one, there exist positive constants $\beta \in$ $(0,1)$ and $\gamma$ such that [1]:

$$
\begin{equation*}
\left\|(B)^{k} y\right\|_{2} \leq \gamma(\beta)^{k}\|y\|_{2} \tag{15}
\end{equation*}
$$

for all $y \in R^{n}$. From equation (13), one obtains [4]:

$$
\begin{equation*}
z(k)=(B)^{k} z(0)+\sum_{j=0}^{k-1}(B)^{k-j-1} N(z(j), w(j)) \tag{16}
\end{equation*}
$$

and therefore:

$$
\begin{equation*}
\|z(k)\|_{2} \leq \gamma(\beta)^{k}\|z(0)\|_{2}+\sum_{j=0}^{k-1} \gamma L(\beta)^{k-j-1}\|z(j)\|_{2} \tag{17}
\end{equation*}
$$

or:

$$
\begin{equation*}
(\beta)^{-k}\|z(k)\|_{2} \leq \gamma\left\{\|z(0)\|_{2}+\sum_{j=0}^{k-1} L(\beta)^{-j-1}\|z(j)\|_{2}\right\} \tag{18}
\end{equation*}
$$

Applying Gronwall-Bellman's inequality [4], it can be deduced that:

$$
\begin{align*}
(\beta)^{-k}\|z(k)\|_{2} & \leq\|z(0)\|_{2} \prod_{j=0}^{k-1}\left(1+\gamma L(\beta)^{-1}\right) \Rightarrow \\
(\beta)^{-k}\|z(k)\|_{2} & \leq\|z(0)\|_{2}(\beta)^{-k}(\beta+L \gamma)^{k} \Rightarrow \\
\|z(k)\|_{2} & \leq(M)^{k}\|z(0)\|_{2} \Rightarrow \\
\|x(k)-\pi(w(k))\|_{2} & \leq(M)^{k}\|x(0)-\pi(w(0))\|_{2} \quad \tag{19}
\end{align*}
$$

where $M=\beta+L \gamma$. Since $L$ can be made arbitrarily small, let us choose: $L<\frac{1-\beta}{\gamma}$ so that $0<M<1$, and the proof is complete.

Theorem 2 states that, as time tends to infinity, any trajectory of (1)-(2) starting at a point sufficiently close to the origin converges to a trajectory that lies entirely on the invariant manifold $S$. Therefore, the long-term asymptotic response of the nonlinear process (1) in the presence of the $w$-dynamics (2) is given by:

$$
\begin{equation*}
x(k) \approx_{k \rightarrow \infty} \pi(w(k)) \tag{20}
\end{equation*}
$$

where $\pi(w)$ is the unique solution to the associated system of invariance NFEs (4). Equivalently, the invariant manifold $S(7)$ is rendered locally attractive $[1,15]$.

## A. Special Case: The Long-Term Dynamic Behavior of Linear Discrete-Time Processes

Let us now consider a linear (linearized) system:

$$
\begin{equation*}
x(k+1)=B x(k)+C w(k) \tag{21}
\end{equation*}
$$

and $w \in R$ a time-varying scalar process parameter following the first-order dynamics:

$$
\begin{equation*}
w(k+1)=a w(k) \tag{22}
\end{equation*}
$$

with $B, C$ being constant matrices with appropriate dimensions and $|a|<1$ (stability assumption for the $w$ dynamics). Notice that one may envision a case where a chemical reaction system with $x$ being the composition vector (in deviation form from the reference steady state conditions), and $w$ the catalyst activity corresponding to a specific deactivation mechanism, is modelled by (21)-(22) [5]. In this case, the objective is to determine the longterm dynamic behavior of process (21) in the presence of catalyst deactivation (22), and therefore, to investigate the possibility of catalyst replacement if conversion or selectivity are affected in an adverse manner. It is assumed that the eigenspectrum of matrix $B$ is comprised of eigenvalues $\lambda_{i}$ with $\left|\lambda_{i}\right|<1, i=1, \ldots, n$, and therefore the discrete-time process (21) is assumed to be a stable one (or stabilized via controller action). Furthermore, it is assumed that the timeconstant associated with the catalyst activity $w$-dynamics is larger compared to the dominant process time-constant (such as in catalyst deactivation due to poisoning [5]) :

$$
\begin{equation*}
|a| \gg \rho \tag{23}
\end{equation*}
$$

where $\rho=\max _{i}\left|\lambda_{i}\right|,(i=1, \ldots, n)$ is the spectral radius of $B$. One may now explicitly calculate the long-term asymptotic process response by solving the system of linear difference equations (21)-(22):

$$
\begin{align*}
x(k) & =B^{k} x(0)+\sum_{i=0}^{k-1} B^{k-i-1} C a^{i} w(0)= \\
& =B^{k} x(0)-w(0)\left\{a^{k} I-B^{k}\right\}(B-a I)^{-1} C(24) \tag{24}
\end{align*}
$$

where the following matrix identity was used:

$$
\begin{equation*}
\sum_{j=0}^{k-1} B^{k-j-1} a^{j}=\left\{B^{k}-a^{k} I\right\}(B-a I)^{-1} \tag{25}
\end{equation*}
$$

Under assumption (23), it can be easily inferred that the longterm asymptotic process response is given by:

$$
\begin{equation*}
x(k) \approx_{k \rightarrow \infty}-w(0)(B-a I)^{-1} C a^{k} \tag{26}
\end{equation*}
$$

Notice, that in the linear case (21)-(22) the associated system of invariance NFEs (4) takes the following form:

$$
\begin{align*}
\pi(a w) & =B \pi(w)+C w \\
\pi(0) & =0 \tag{27}
\end{align*}
$$

Under the assumptions of Theorem 1, the above system of NFEs admits a unique solution: $\pi(w)=\Pi w$, where $\Pi$ is the unique solution that satisfies the following Lyapunov matrix equation:

$$
\begin{equation*}
\Pi a I-B \Pi=C \tag{28}
\end{equation*}
$$

It is easy to show that (28) admits the following solution:

$$
\begin{equation*}
\Pi=-(B-a I)^{-1} C \tag{29}
\end{equation*}
$$

where $(B-a I)$ is indeed an invertible matrix since $a$ does not belong to the eigenspectrum of the process characteristic matrix B, which is guaranteed by Lemma 1 and Theorem 1. According to Theorem 2, the invariant manifold $x=\Pi w$ is locally attractive, and the long-term asymptotic behavior of the chemical reaction system (21) in the presence of catalyst deactivation (22) is given by:

$$
\begin{equation*}
x(k) \approx_{k \rightarrow \infty} \Pi w(k)=-w(0)(B-a I)^{-1} C a^{k} \tag{30}
\end{equation*}
$$

The above expression was derived on the basis of the invariant manifold construction of the proposed approach, and it coincides with the one (Eq. (26)) obtained through a direct calculation of the solution of the discrete-time linear process dynamic equations (21)-(22).

## IV. Illustrative Example

Immobilized cell and enzyme bioreactors are now widely used in a variety of interesting applications. In these systems, the short-term behavior of the bioreactor is dependent upon the nonlinear kinetics of the immobilized enzymes or cells participating in the reactions. However, the long-term behavior of the bioreactors depends upon the stability of the immobilized enzymes or the viability of the immobilized cells. The short term behavior of these systems are important in determining the conversion of a nutraceutical or degradation of a toxin for example, parameters that define the performance of the bioreactor. The long term behavior of the bioreactor will determine when the enzyme or cell catalyst needs to be replaced to maintain conversions at acceptable levels. Therefore, accurately estimating when bioreactor performance declines below acceptable levels has important consequences for the profitability of a process or the health of a patient.

Actual kinetic data on enzyme performance and enzyme degradation are considered in the present study, obtained from previous work by Hill and coworkers [13] for an immobilized enzyme bioreactor for the production of food grade linoleic acid from corn oil. There is one enzymatic step for the reaction described, however, multiple enzymatic steps are necessary for the conversion of corn oil to the desired nutraceutical, conjugated linoleic acid [13]. In order to illustrate and evaluate the proposed method, we have included a second enzymatic step in our example and used kinetic parameters for the second enzyme that were assumed to be representative. In the example, we assume that the
enzymatic bioreactor behaves as an ideal continuous stirred tank reactor (CSTR). It is also assumed that the first enzyme converts substrate into product, in this case corn oil into linoelic acid, via a ping-pong bi bi mechanism, as reported in [13]. The second enzyme converts substrate to product via a Michaelis-Menten mechanism, and both enzymes degrade via a first order decomposition process. The following nonlinear dynamic process model is considered:

$$
\begin{align*}
& \frac{d S}{d t}=f^{(1)}\left(S, E_{1}, E_{2}\right) \\
&+\frac{v_{0}}{}=\frac{k_{1} S}{1-k_{2} S}+\frac{k_{3} E_{2} S}{K_{M_{2}}+S}+ \\
& \frac{d E_{1}}{d t}=g^{(1)}\left(E_{1}, E_{2}\right)=-k_{d 1} E_{1} \\
& \frac{d E_{2}}{d t}=g^{(2)}\left(E_{1}, E_{2}\right)=-k_{d 2} E_{2} \tag{31}
\end{align*}
$$

The above dynamic equations describe the change in substrate concentration in the reactor as a function of time, and the degradation of activity of the two enzymes. $S$, $S_{0}(=3.4 M), E_{1}$ and $E_{2}$ represent the concentrations of substrate, substrate in the feed stream, enzyme one, and enzyme two respectively. $k_{1}\left(=8.2 * 10^{-2} h^{-1} g^{-1}\right), k_{2}(=$ $\left.5.9 * 10^{-1} M^{-1}\right), k_{3}\left(=3 * 10^{-1} M h^{-1} g^{-1}\right)$, and $K_{M_{2}}(=$ $8 M)$ represent kinetic parameters describing the rates of reaction of enzyme one and two, and $k_{d 1}\left(=3.4 * 10^{-3} h^{-1}\right)$ and $k_{d 2}\left(=5 * 10^{-4} h^{-1}\right)$ are kinetic parameters describing the rate of deactivation of enzymes one and two respectively. $v_{0}(=100 \mathrm{ml} / \mathrm{h})$ is the flow rate of the substrate and $V(=$ 50 ml ) is the reactor volume. Using a time-discretization step: $\delta=0.01 h$ which is smaller than the dominant process timeconstant, Euler's discretization method was applied in order to obtain a quite accurate discrete-time dynamic process model:

$$
\begin{align*}
& S(k+1)=F^{(1)}\left(S(k), E_{1}(k), E_{2}(k)\right)= \\
= & S(k)+f^{(1)}\left(S(k), E_{1}(k), E_{2}(k)\right) \delta \\
& E_{1}(k+1)=G^{(1)}\left(E_{1}(k), E_{2}(k)\right)= \\
= & E_{1}(k)+g^{(1)}\left(E_{1}(k), E_{2}(k)\right) \delta \\
& E_{2}(k+1)=G^{(2)}\left(E_{1}(k), E_{2}(k)\right)= \\
= & E_{2}(k)+g^{(2)}\left(E_{1}(k), E_{2}(k)\right) \delta \tag{32}
\end{align*}
$$

In order to conform to the theory presented in previous sections, the following set of deviation variables relative to the equilibrium point $\left(S^{0}, E_{1}^{0}, E_{2}^{0}\right)=(3.4,0,0$,$) are$ introduced:

$$
\begin{align*}
x_{1} & =S-S^{0} \\
w_{1} & =E_{1}-E_{1}^{0} \\
w_{2} & =E_{2}-E_{2}^{0} \tag{33}
\end{align*}
$$

Let us also denote: $\bar{F}^{(1)}\left(x_{1}, w_{1}, w_{2}\right)=F^{(1)}\left(x_{1}+S^{0}, w_{1}+\right.$ $\left.E_{1}^{0}, w_{2}+E_{2}^{0}\right), \bar{G}^{(i)}\left(w_{1}, w_{2}\right)=G^{(i)}\left(w_{1}+E_{1}^{0}, w_{2}+E_{2}^{0}\right)$ ( $i=1,2$ ). Notice that for the bioreactor model (32) all conditions of Theorems 1 and 2 are satisfied. Therefore,
there exists a unique and locally analytic invariant manifold: $x_{1}=\pi\left(w_{1}, w_{2}\right)$, with $\pi\left(w_{1}, w_{2}\right)$ being the solution of the following nonlinear functional equation:

$$
\begin{align*}
\pi\left(\bar{G}^{(1)}\left(w_{1}, w_{2}\right), \bar{G}^{(2)}\left(w_{1}, w_{2}\right)\right) & =\bar{F}^{(1)}\left(\pi\left(w_{1}, w_{2}\right), w_{1}, w_{2}\right) \\
\pi(0,0) & =0 \tag{34}
\end{align*}
$$

A series solution of the above functional equation is sought around the origin. The Taylor coefficients of the unknown solution $x_{1}=\pi\left(w_{1}, w_{2}\right)$ can be automatically computed by using a simple MAPLE code. In particular, a third-order series truncation is considered leading to the following thirdorder Taylor polynomial approximation of the actual solution:

$$
\begin{align*}
& x_{1}=\pi^{[3]}\left(w_{1}, w_{2}\right)=-0.13880 w_{1}+0.04474 w_{2}- \\
- & 0.00564\left(w_{1}\right)^{2}+0.00053 w_{1} w_{2}+0.00041\left(w_{2}\right)^{2}- \\
- & 0.00068\left(w_{1}\right)^{3}+0.00025\left(w_{1}\right)^{2} w_{2}- \\
- & 0.000015 w_{1}\left(w_{2}\right)^{2}+0.000002\left(w_{2}\right)^{3} \tag{35}
\end{align*}
$$

Therefore, according to Theorem 2, the long-term asymptotic behavior of the bioreactor (32) can be calculated by using the following formula:

$$
\begin{array}{rll}
x_{1}(k) & \approx_{k \rightarrow \infty} & \pi^{[3]}\left(w_{1}(k), w_{2}(k)\right) \approx \\
& \approx_{k \rightarrow \infty} & \pi^{[3]}\left(4(0.99966)^{k},(0.99995)^{k}\right) \tag{36}
\end{array}
$$

Both the actual dynamic response of the bioreactor was computed by simulating the full process model (32), as well as the long term asymptotic behavior of the bioreactor by using equation (36). As it can be seen in Figure 1, the estimated substrate concentration at the outlet of the reactor obtained through equation (36) is indistinguishable from the actual substrate concentration at times larger than 150 h , the approximate half life of the fastest decaying enzyme.

Acknowledgement Financial support from the National Science Foundation through Grant CTS-0131809 is gratefully acknowledged by the first author.

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