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## A model-based characterization of the long-term asymptotic behavior of nonlinear discrete-time processes using invariance functional equations

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#### **Abstract**

The present research work proposes a new approach to the problem of quantitatively characterizing the long-term dynamic behavior of nonlinear discrete-time processes. It is assumed that in order to analyze the process dynamic behavior and digitally simulate it for performance monitoring purposes, the discrete-time dynamic process model considered can be obtained: (i) either through the employment of efficient and accurate discretization methods for the original continuous-time process which is mathematically described by a system of nonlinear ordinary (ODEs) or partial differential equations (PDEs) or (ii) through direct identification methods. In particular, nonlinear processes are considered whose dynamics can be viewed as driven: (i) either by an external time-varying "forcing" input/disturbance term, (ii) by a set of time-varying process parameters or (iii) by the autonomous dynamics of an upstream process. 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 solution is derived. The solution to the aforementioned system of NFEs is then proven to represent a locally analytic invariant manifold of the nonlinear discrete-time process under consideration. 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 with the aid of a symbolic software package such as MAPLE. Under a certain set of conditions, it is shown that the invariant manifold computed attracts all system trajectories, and therefore, the asymptotic process response and long-term dynamic behavior are determined through the restriction of the discrete-time process dynamics on the invariant manifold.

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#### 1. Introduction

The chemical engineering literature is dominated by physical and (bio)chemical processes that exhibit nonlinear behavior and are typically modeled by systems of nonlinear ordinary (ODEs) or partial differential equations (PDEs) in the continuous-time domain, or systems of nonlinear difference equations (DEs) in the discrete-time domain (Bequette,

1998; Christofides, 2001; Ogunnaike & Ray, 1994; Ray, 1981). Furthermore, efficient and accurate discrete-time dynamic process modeling techniques have been developed that capitalize on the current availability of enhanced computational capabilities allowing the digital simulation, analysis and characterization of complex process dynamic behavior to be performed in a thorough manner. In particular, the employment of efficient discretization techniques for the system of ODEs or PDEs that describe the behavior of the process of interest in the continuous-time domain, as well as various process identification methods, can lead to discrete-time dynamic process models characterized by a high degree of fidelity and amenability to insightful theoretical and

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computational investigations on the process dynamic behavior. However, despite the fact that the dynamic analysis of linear processes can be performed with rigor (Bequette, 1998; Elaydi, 1999; Ray, 1981), it still remains a rather challenging task for nonlinear processes, and it undoubtedly represents an area of considerable research effort. 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 traditionally 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 (Arnold, 1983; Carr, 1981; Cox & Roberts, 1995; Foias, Jolly, Kevrekidis, Sell, & Titi, 1989; Foias, Sell, & Titi, 1989; Guckenheimer & Holmes, 1983; Kaper, Koppel, & Jones, 1996; Moore, 1995; Roberts, 1997; Wiggins, 1990). 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. A representative, and certainly not exhaustive, sample of recent applications of invariant manifold theory to chemical reaction systems for model-reduction purposes can be found in Balakotaiah and Dommeti (1999), Gorban and Karlin (2003), Kumar, Christofides, and Daoutidis (1998), Li and Rabitz (1994), Rhodes, Morari, and Wiggins (1999), Vora and Daoutidis (2001) and Zmievski, Karlin, and Deville (2000). Furthermore, the study of invariant manifolds has been historically conducted in connection with the existence problem of (un)stable and center manifolds, stability, as well as bifurcation analysis (Wiggins, 1990). 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) (Wiggins, 1990). The latter requirement, while always achievable through a coordinate transformation, may result in a computationally demanding numerical problem particularly for higher order systems, such as the ones obtained from discretization or modal decomposition techniques applied to distributed parameter systems (Christofides, 2001). In the same spirit as the standard stable and center manifold theory, conceptual and technical extensions have been developed in the case of singularly perturbed systems, where the classification of the corresponding invariant manifolds as slow and fast is a natural consequence of the two-time scale separation property (Fenichel, 1979; Kokotovic, Khalil, & O'Reilly, 1986). 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 under the name inertial manifold (Christofides, 2001). It should be pointed out that unlike the well-known existence theorems in the standard stable and center manifold theory (Wiggins, 1990), inertial manifolds were proven to exist only for certain classes of parabolic PDEs (on a case-by-case basis). However, there are systematic techniques available for computing, up to a desired degree of accuracy, approximations of the aforementioned solutions based on the so-called manifold equation (Christofides, 2001).

Finally, research results on symmetry-induced generalized invariants for distributed parameter systems were also reported in Palazoglu and Karakas (2000).

The present research work proposes a new systematic approach to the problem of quantitatively characterizing the long-term dynamic behavior of nonlinear discrete-time processes. In particular, nonlinear processes are considered whose dynamics can be viewed as driven: (i) either by an external time-varying "forcing" input/disturbance term, (ii) by a set of time-varying process parameters or (iii) by the autonomous dynamics of an upstream process. 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 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 represent a locally analytic invariant manifold map of 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 (Wiggins, 1990). Furthermore, the local analyticity property of the invariant manifold map enables the development of a series solution method, which can be easily implemented using MAPLE. Under a certain set of conditions, it can be shown that the invariant manifold computed attracts all system trajectories, and therefore, the asymptotic process response and long-term dynamic behavior are calculated through the restriction of the discrete-time process dynamics on the invariant manifold.

The present paper is organized as follows: Section 2 contains some mathematical preliminaries that are necessary for the ensuing theoretical developments. The paper's main results are presented in Section 3, accompanied by remarks and comments on their potential use for process performance monitoring purposes. An illustrative case study of an enzymatic bioreactor is presented in Section 4, followed by a few concluding remarks in Section 5.

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