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Uncertainty quantification in stability analysis of chaotic systems with discrete delays

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ABSTRACT

Time delay is ubiquitous in many real-world physical and biological systems. It typically gives rise to rich dynamic behaviors, from aperiodic to chaotic. The stability of such dynamic behaviors is of considerable interest for process control purposes. While stability analysis under deterministic conditions has been extensively studied, not too many works addressed the issue of stability under uncertainty. Nonetheless, uncertainty, in either modeling or parameter estimation, is inevitable in complex system studies. Even for high-fidelity models, the uncertainty of input parameters could lead to divergent behaviors compared to the deterministic study. This is especially true when the system is at or near the bifurcation point. To this end, we investigated generalized polynomial chaos (GPC) to quantify the impact of uncertain parameters on the stability of delay systems. Our studies suggested that uncertainty quantification in delay systems provides richer information for system stability compared to deterministic analysis. In contrast to the robust yet time-consuming Monte Carlo or Latin hypercube sampling method, GPC approach achieves the same accuracy but only with a fraction of the computational overhead.

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1. Introduction

One of the grand challenges in the study of complex system behavior is the time delay effect [1]. In fact, time delay is ubiquitous and inherent in a plethora of physical and biological systems, from manufacturing to transportation, ecology and neural science, among others [2]. Common causes for time delay in control engineering include the limited communication capacity and finite communication speed, as sensors and actuators are rarely collocated in control systems. For instance, in steel rolling process, the thickness sensor is usually positioned at a certain distance away from the rolling gap, leading to measurement delay of the thickness, which is consequently used in a feedback control scheme [3]. In the study of glucose-insulin regulatory system, a time delay model is often used to describe the interaction of glucose, insulin and glucose-insulin mixture, to account for the delay effect (~30–45 minutes) of insulin on glucose production [4] for effective and personalized treatment. Notably, time delay can give rise to complicated dynamic behaviors even in simple systems. As such, when the time delay for transcription and translation is considered, even simple regulatory gene circuit can dramatically alter the course of system evolution and exhibit rich steady-state behaviors, including limit cycle, aperiodic, weak/strong chaotic, and even intermittent patterns [5]. Hence, time delay dynamic model is promising to represent the complex gene regulatory system with a myriad of gene circuits and pinpoint gene expressions associated with certain diseases.

Delay differential equations (DDEs) are among the most prevalent tools to describe those dynamic systems with time delay. In DDEs, the evolution of the variable of interest $y(t)$ depends on its state at present time t as well as $t-\tau$ in the past, which makes it non-Markovian, as indicated in Eq. (1) for a linear scalar system with a single discrete delay,

$$\dot{y}(t) = ay(t) + by(t-\tau). \tag{1}$$

Similar to ordinary differential equations (ODEs), the solution to DDEs can be derived via the characteristic equations. Here, the linear scalar DDE in Eq. (1) has transcendental characteristic equation

$$-\lambda + a + be^{-\lambda\tau} = 0, \tag{2}$$

where λ is called the characteristic root or eigenvalue. The solution set is often referred to as the spectrum, which bears the biomarkers of the underlying dynamic systems. Remarkably, the presence of exponential term $e^{-\lambda\tau}$ in Eq. (2) leads to an infinite number of possible values of λ, consequently an infinite number of solutions. In other words, the underlying dynamics is embedded in an infinite-dimensional phase space. Therefore, this delay term renders solutions of DDEs differ from that of ODEs in a striking manner. It crucially affects the behavior of complex systems, leading to

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a complicated trajectory of dynamics and even chaotic motion [6], and poses tremendous challenges to study local stability of equilibria of such systems, one of the key issues in dynamic systems.

While stability analysis of dynamic systems with delay has been extensively explored [7–9], the performance under uncertainty has not been well investigated. Nonetheless, just like any real-world complex systems, those delay systems are not immune to a wide range of uncertainty in modeling, initial and boundary conditions as well as model parameter calibration. Therefore, there is a pressing need to quantify such uncertainty for reliable feedback control or robust process optimization. While Monte Carlo (MC) simulation is the most prevalent method to quantify uncertainties, it inevitably leads to immense computational cost due to the large number of samples required [10]. This has stymied its application in critical settings such as real-time feedback control. On the other hand, effective sampling approaches have been studied, including quasi-Monte Carlo (QMC) [11] and space filling design algorithms (e.g., variations of Latin hypercube design [12,13]). QMC capitalizes on a low-discrepancy sequence for faster rate of convergence, compared to the pseudorandom sequence in MC, and may only marginally save computational budget. Latin hypercube design (LHD) largely hinges on the quality and quantity of sampling points. As an alternative, general polynomial chaos (GPC) [14] is a spectral expansion method and independent of the sampling points, conducive for large-scale simulations. To this end, we investigated the stability of delay systems under uncertainty using GPC. The focus of this present research is only on the parameter uncertainty in systems with single discrete delay, but it is applicable to general continuous time delays.

2. Stability analysis of DDEs

Stability of DDEs have been extensively studied in literature, using a variety of approaches, including Laplace transform [15], Lyapunov functions [16], perturbation analysis [17], Lambert W functions [7,18], semi-discretization [8], and Galerkin approximation [9]. Whereas other models mentioned here suffers from the intricate mathematical formulations, Lambert W function is of particular interest for first order DDEs, whose characteristic equation has the explicit form of mapping $we^w \mapsto z$ for scalar $w,\ z \in \mathbb{C}$ (set of complex numbers). As such, the eigenvalues can be solved in a straightforward way using the Lambert function W, satisfying $w = W(z)$, the inverse of the mapping $we^w \mapsto z$ [7]. It has an infinite number of branches $W_k(z) = \{w \in \mathbb{C} : we^w = z\}$, $k = 0,\ \pm 1, \pm\ 2,\ \pm 3, \ldots$ [19], corresponding to the infinite number of solutions for the DDE in Eq. (1). Concretely, the characterization equation in Eq. (2) can be reformulated as

$$(\lambda - a)\tau e^{(\lambda - a)\tau} = b\tau e^{-a\tau}. \tag{3}$$

That is, $w = (\lambda - a)\tau$ and $z = b\tau e^{-a\tau}$. Therefore, eigenvalues $\lambda_k = \frac{W_k(b\tau e^{-a\tau})}{\tau} + a$. The stability is determined upon the principal branch at $k = 0$, namely, $\lambda_0 = \frac{W_0(b\tau e^{-a\tau})}{\tau} + a$. The dynamic evolution is unstable, if λ_0 lies to the right of the imaginary axis, i.e., $Re(\lambda_0) > 0$.

For the second or higher order DDEs, matrix Lambert W function has recently been developed, which registered comparable stability chart to that obtained using bifurcation analysis [7]. Although the matrix Lambert W function is conceptually easy to understand, as it resembles the state transition matrix in linear ODEs, it is only restricted to a certain class of DDEs and the mathematical formulation is usually cumbersome. Thus, discretization and semi-discretization approaches have been developed to approximate λ for higher-order DDEs. Among them, temporal finite element method has garnered enormous attentions, for example, in the applications of machining [20].

3. Stability analysis under uncertainty

However, most existing works do not consider the uncertainty associated with modeling and parametrization. Indeed, due to limitations in experimental study or calibration and measurement error, the process parameters cannot be exactly specified and are often modeled as random quantities in a probabilistic framework. The most straightforward way to quantify the impact of such uncertainty on stability is the Monte Carlo (MC) simulation. It is a brute force model in that it relies on large samples from the underlying random distribution. The system behavior is then evaluated as the mean response of those sampled realization, and it is often infeasible due to the overwhelming computational overhead involved. While Latin hypercube design (LHD) [21] tends to optimize the sampling process in MC, it is still a sampling-based approach, and only marginally relieve the computational cost. As a potential remedy for the huge computational overhead involved in sampling-based approaches, generalized polynomial chaos (GPC) expansions have arisen as an efficient alternative to represent stochastic quantities as spectral expansions of orthogonal polynomials [14].

3.1. Generalized polynomial chaos (GPC)

The generalized polynomial chaos (GPC) is based on the original Wiener's theory of homogeneous chaos [22]. A stochastic process $\lambda_0(\xi, t)$ or simply a random variable/function $\lambda_0(\xi)$ with finite second-order moment can be expressed as a convergent series of polynomials, viz., $\lambda_0(\xi,\ t) = \sum_{i=0}^{\infty} c_i(t)\phi_i(\xi)$. Here, ξ is the underlying random variable, $\phi_i(\xi)$ denotes the polynomial series conforming to the distribution of ξ, and c_i is the corresponding coefficient. This spectral expansion offers fast exponential convergence rate, and is a cheap alternative to MC simulations. According to the Wiener–Askey scheme [23], GPC expansion with Hermite polynomial basis has been used effectively to quantify uncertainty with Gaussian inputs, Jacobian polynomials for beta distribution, and so on. The polynomial bases $\phi_i's$ are orthogonal in that

$$\begin{aligned}\langle \phi_i, \phi_j \rangle_{\rho(\xi)} &= E\left[\phi_i(\xi)\phi_j(\xi)\right] = \int \phi_i(\xi)\phi_j(\xi)\rho(\xi)d\xi \\ &= \Delta_i \delta_{ij}, \qquad i, j \in \mathbb{N}\end{aligned} \tag{4}$$

where $\rho(\xi)$ represents the probability density function (PDF) of ξ, and $\langle \cdot,\ \cdot \rangle$ is the inner product operator with respect to $\rho(\xi)$. $\delta_{ij} = \begin{cases} 0, & i \neq j \\ 1, & i = j \end{cases}$ denotes the Kronecker function. The integration in Eq. (4) is oftentimes approximated using Gaussian quadrature rules. With N quadrature points and weights $\{(\xi^{(k)},\ \omega^{(k)}) : k = 1,\ 2,\ \ldots,\ N\}$,

$$\Delta_i = \sum_{k=1}^{N} \omega^{(k)} \phi_i\left(\xi^{(k)}\right)\phi_i\left(\xi^{(k)}\right). \tag{5}$$

The coefficient c_i can be determined by the intrusive stochastic Galerkin [23], in which the variable of interest $\lambda_0(\xi, t)$ is projected onto the polynomial basis $\phi_i(\xi)$ as $\langle \lambda_0(\xi, t), \phi_j \rangle_{\rho(\xi)}$ to minimize the spectral expansion approximation (see Section 4 for details). Therefrom, the distribution of $\lambda_0(\xi, t)$ can be characterized as $E[\lambda_0(\xi, t)] = \Delta_0$ and $\mathrm{var}(\lambda_0(\xi, t)) = \sum_{i=1}^{\infty} [c_i(t)]^2 \Delta_i$ [23].

3.2. Maximum entropy method

Further, we are more interested in the distribution of λ_0 and $P(\lambda_0) > 0$ in the stability analysis. To this end, we extracted the first four raw moments from GPC representation, and adopted the maximum entropy principle (MEP) [24] to estimate the PDF $f_{\lambda_0}(\lambda_0)$ of