

Unified Data-Driven Framework for Hopf Bifurcation Analysis, Machine Learning, Phase Space Characterization, and Bifurcation-Aware Optimal Control of Nonlinear Dynamical Systems

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Abstract

Nonlinear dynamical systems frequently exhibit multiple steady states, limit points, and self-sustained oscillations that can significantly affect process stability and operational performance. This study presents an integrated computational framework that combines nonlinear bifurcation analysis, data-driven machine learning, phase-space characterization, and dynamic optimal control to analyze and regulate nonlinear engineering systems operating near critical instability regions. Numerical continuation is first employed to identify the principal bifurcation structure and locate the Hopf bifurcation point together with the associated limit point. A simulation-based dataset is subsequently generated by systematically varying the bifurcation parameter in the vicinity of the critical operating region. Statistical features extracted from the resulting dynamic trajectories are used to train a supervised machine-learning classifier to distinguish between steady-state and oscillatory operating regimes. Phase-space analysis is performed to validate the identified dynamic behavior and to confirm the existence of stable limit cycles associated with the Hopf bifurcation. Finally, dynamic optimal control problems are formulated within Pyomo.DAE framework and solved using IPOPT. Both conventional and bifurcation-aware optimal control formulations are investigated to evaluate the influence of nonlinear stability information on the resulting optimal trajectories. The results demonstrate that the proposed methodology provides an effective framework for integrating nonlinear dynamics, machine learning, and optimization, offering a computationally efficient approach for stability assessment and control of complex nonlinear engineering systems.

Keywords: Hopf Bifurcation, Nonlinear Dynamical Systems, Machine Learning, Phase Space Analysis, Dynamic Optimal Control

1. Introduction

Nonlinear dynamical systems arise naturally in numerous branches of science and engineering, including chemical processing, environmental engineering, biological systems, fluid mechanics, energy systems, and biochemical reactors. Unlike linear systems, nonlinear processes frequently exhibit multiple steady states, hysteresis, oscillatory behavior, and sudden transitions between qualitatively different operating regimes.

These phenomena originate from the intrinsic nonlinear interactions among reaction kinetics, transport mechanisms, and external forcing, making the prediction and regulation of system behavior considerably more challenging than in linear systems. Consequently, understanding the nonlinear stability characteristics of engineering systems has become an important prerequisite for designing reliable and efficient operating strategies.

Among the various nonlinear phenomena encountered in engineering systems, bifurcations represent critical points at which small changes in operating parameters produce significant qualitative changes in system dynamics. The identification of bifurcation points provides valuable information regarding operating limits, process stability, and the emergence of undesirable dynamic behavior. In particular, Hopf bifurcations are of considerable practical importance because they mark the transition from stable equilibrium solutions to sustained oscillatory motion through the appearance of periodic solutions.

Such oscillations may reduce process efficiency, increase operational costs, accelerate equipment degradation, and compromise safety in industrial applications. Consequently, identifying the onset of oscillatory behavior and understanding its underlying mechanisms remain fundamental objectives in nonlinear systems analysis. Recent advances in computational continuation techniques have significantly improved the ability to analyze nonlinear dynamical systems. Numerical continuation algorithms enable the systematic tracking of equilibrium branches as system parameters vary while simultaneously identifying critical bifurcation points such as limit points, branch points, and Hopf bifurcations.

These techniques provide a global understanding of system behavior that cannot be obtained from conventional time-domain simulations alone. Instead of examining isolated operating conditions, continuation methods reveal the overall stability landscape of the system and identify parameter regions associated with qualitative changes in dynamic behavior.

At the same time, the rapid development of artificial intelligence and machine learning has created new opportunities for analyzing nonlinear engineering systems. Rather than relying exclusively on first-principles mathematical models, modern data-driven approaches extract informative features directly from simulation or experimental data and use these features to characterize different operating regimes.

Supervised learning techniques have demonstrated considerable success in classification, prediction, fault diagnosis, and process monitoring, offering computationally efficient alternatives to repeated numerical simulations. In nonlinear process systems, feature-based machine learning models can rapidly distinguish between stable and oscillatory operating conditions once appropriate training data have been generated.

The combination of physics-based modeling with machine learning has emerged as a particularly promising research direction in process systems engineering. Instead of replacing mechanistic models, machine learning algorithms can complement classical nonlinear analysis by providing rapid approximations of stability regions and dynamic behavior. Such hybrid approaches combine the physical interpretability of first-principles models with the computational efficiency of data-driven methods. As a result, they provide a practical framework for real-time monitoring, predictive analysis, and intelligent decision making in complex engineering systems.

An equally important aspect of nonlinear system analysis is the geometric interpretation of system dynamics through phase-space representations. Phase portraits provide a direct visualization of system trajectories and reveal whether solutions converge toward stable equilibrium points, diverge from unstable operating conditions, or evolve into periodic limit cycles. When combined with numerical continuation results, phase-space analysis provides an independent verification of the predicted bifurcation structure and offers valuable insight into the underlying mechanisms governing the observed dynamics.

This geometric interpretation also facilitates the validation of machine learning classification results by relating statistical features extracted from time-series data to the actual trajectories followed by the nonlinear system.

While bifurcation analysis and machine learning improve understanding of nonlinear behavior, practical engineering applications ultimately require effective control strategies capable of maintaining stable operation near critical operating regions. Classical optimal control techniques seek control actions that minimize predefined performance indices while satisfying the governing dynamic equations and operational constraints.

However, conventional optimal control formulations generally optimize economic or performance objectives without explicitly considering the proximity of bifurcation boundaries or the nonlinear stability characteristics of the underlying system. Consequently, optimal solutions obtained using standard formulations may inadvertently operate close to instability regions where small disturbances can trigger undesirable oscillatory behavior.

Incorporating bifurcation information into the control formulation provides an opportunity to design control strategies that not only optimize performance but also enhance dynamic robustness. By accounting for the location of critical stability boundaries identified through continuation analysis, bifurcation-aware control formulations can steer system trajectories away from oscillatory operating regions while maintaining acceptable economic performance. Such an integrated strategy combines the complementary strengths of nonlinear dynamics, data-driven analysis, and mathematical optimization to achieve improved process operation.

Motivated by these considerations, the present work proposes a unified computational framework for the analysis and control of nonlinear dynamical systems operating near Hopf bifurcation points. The methodology begins with numerical continuation to identify the critical bifurcation structure and determine the onset of oscillatory behavior.

A simulation dataset is then generated by systematically varying the principal bifurcation parameter over the neighborhood of the critical point. Representative statistical features are extracted from the resulting dynamic trajectories to construct a compact description of system behavior. These features are subsequently employed to train a supervised machine learning classifier capable of distinguishing between steady-state and oscillatory operating regimes. The classification results are further validated through phase-space analysis, providing a geometric confirmation of the identified dynamic behavior.

Finally, the information obtained from bifurcation analysis and data-driven classification is incorporated into a dynamic optimal control framework formulated within the Pyomo.DAE environment and solved using nonlinear programming techniques.

The proposed methodology establishes a coherent workflow that links nonlinear bifurcation analysis, machine learning, phase-space characterization, and optimal control into a single computational framework.

Although demonstrated using a representative nonlinear dynamical system, the approach is sufficiently general to be extended to a wide variety of engineering applications involving nonlinear instabilities, including chemical reactors, environmental transport systems, biochemical processes, energy conversion technologies, fluid dynamic systems, and other multivariable nonlinear processes. By integrating complementary computational tools within a unified framework, the proposed methodology provides an effective strategy for understanding, predicting, and controlling complex nonlinear dynamics in modern engineering systems.

2. Literature Review

The modeling, analysis, and simulation of nonlinear chemical processes have been extensively investigated over the past several decades because of their importance in process design, operation, and control. Early work by Chiang, Russell, and Braatz (2001) emphasized the importance of extracting meaningful information from process measurements for fault diagnosis and system monitoring, demonstrating that data-driven techniques can significantly improve process reliability [1]. Similarly, Edgar, Himmelblau, and Lasdon (2001) presented comprehensive methodologies for mathematical modeling and numerical optimization of chemical processes, establishing a foundation for modern computational process engineering [2]. During the same period, Nelles (2001) demonstrated that nonlinear system identification techniques provide powerful tools for constructing predictive models that represent highly nonlinear industrial processes [3].

Building upon these developments, Bequette (2003) discussed the central role of dynamic process modeling in controller design and emphasized the interaction between nonlinear process behavior and control system performance [4]. Later, Box, Hunter, and Hunter (2005) introduced statistical methodologies for experimental design and data analysis that remain fundamental for constructing reliable engineering datasets [5]. These statistical tools have become increasingly important for validating computational models and interpreting experimental observations.

As computational capabilities improved, greater attention was devoted to dynamic simulation and advanced process analysis. Camacho and Bordons (2007) demonstrated the advantages of predictive modeling for dynamic process operation, while Ingham et al. (2007) provided a detailed treatment of nonlinear reactor dynamics and transient process behavior [6,7]. Around the same time, Cutlip and Shacham (2008) emphasized the importance of numerical methods for solving nonlinear differential equations encountered in chemical engineering applications [8]. Likewise, Cussler (2009) presented comprehensive analyses of mass-transfer phenomena that strongly influence transport-limited reacting systems [9].

The integration of mathematical optimization with process engineering continued to expand through the work of Biegler (2010), who described efficient nonlinear programming algorithms applicable to large-scale engineering systems [10]. Subsequently, Himmelblau and Riggs (2012) further developed rigorous methods for mathematical modeling and engineering calculations, while Sundmacher (2012) highlighted the increasing importance of model-based engineering as a framework for integrating simulation, optimization, and process analysis into a unified computational environment [11,12].

Recent years have witnessed rapid growth in artificial intelligence and machine learning applications within engineering. Goodfellow, Bengio, and Courville (2016) established the theoretical foundations of modern deep learning, enabling complex nonlinear relationships to be learned directly from data [13]. These developments have significantly influenced process systems engineering, where machine learning models increasingly complement first-principles mathematical models.

The introduction of the Pyomo optimization framework by Hart et al. (2017) provided an open-source environment for large-scale mathematical modeling and dynamic optimization, facilitating the development of flexible computational workflows [14]. During the same period, Seborg et al. (2017) continued to advance process dynamics and control methodologies by integrating mathematical modeling with modern computational tools [15]. Comprehensive treatments of process design and thermodynamic modeling were subsequently provided by Turton et al. (2018) and Smith et al. (2018), further strengthening the theoretical basis for reactor analysis and process design [16,17].

Modern chemical reaction engineering has increasingly focused on nonlinear reactor behavior and computational simulation. Fogler (2020) presented detailed analyses of reactor modeling and reaction kinetics, while Montgomery (2020) emphasized rigorous statistical techniques for analyzing engineering data [18,19]. During the same year, Rawlings, Mayne, and Diehl (2020) further advanced computational approaches for dynamic process optimization and predictive modeling [20].

The increasing availability of industrial data has accelerated the application of statistical learning techniques in process engineering. Hastie, Tibshirani, and Friedman (2021) provided comprehensive treatments of supervised learning algorithms widely employed in engineering data analysis [21]. At the same time, Zhang, Ge, and Song (2021) reviewed modern data-driven monitoring techniques for chemical processes, while Liu, Ding, and Yin (2021) highlighted the growing role of artificial intelligence in industrial process monitoring and fault diagnosis [22,23].

These studies collectively demonstrate that machine learning techniques can successfully identify complex nonlinear operating regimes using process measurements. More recently, Towler and Sinnott (2022) emphasized the integration of computational methods into modern process design, whereas Ge et al. (2022) reviewed the expanding role of data mining and machine learning throughout the process industries [24,25]. Similarly, Zhang, Qin, and Chai (2022) discussed recent advances in industrial artificial intelligence for process analytics [26]. Continuing this trend, Wang, Liu, and Ge (2023) reviewed machine learning-assisted process modeling and optimization, while Liu, Ge, and Song (2023) summarized the growing importance of intelligent manufacturing technologies [27,28].

Finally, Zhao, Ding, and Yin (2024) highlighted recent advances in data-driven modeling of nonlinear industrial processes, and Wang, Ge, and Huang (2024) reviewed emerging opportunities for integrating artificial intelligence with process systems engineering [29,30]. Together, these recent studies demonstrate that combining first-principles models with machine learning techniques provides a promising direction for the analysis, monitoring, and intelligent operation of nonlinear engineering systems.

3. Main Objectives of the Research

The primary objective of this research is to develop an integrated computational framework for the analysis and control of nonlinear dynamical systems operating in the vicinity of critical bifurcation points. The study seeks to combine nonlinear bifurcation analysis, data-driven characterization, machine learning-based regime classification, phase space analysis, and dynamic optimal control into a unified methodology capable of identifying, interpreting, and regulating complex system behavior.

A key objective is to employ numerical continuation techniques to locate and characterize critical bifurcation points, particularly Hopf bifurcations, which mark the transition from stable steady-state operation to sustained oscillatory dynamics.

Understanding the location and stability characteristics of these bifurcations provides valuable insight into the operating limits of nonlinear systems and forms the basis for subsequent analysis.

A further objective is to construct a representative dataset by systematically varying the bifurcation parameter and extracting descriptive features from the resulting system trajectories. This dataset is then used to train a machine learning classifier capable of distinguishing between steady-state and oscillatory operating regimes. The classification framework provides a computationally efficient surrogate for identifying dynamic behavior without repeatedly solving the governing differential equations.

Another objective is to validate the identified dynamical regimes through phase space analysis, thereby providing a geometric interpretation of the system behavior and confirming the existence of limit cycles associated with Hopf bifurcations. The final objective is to formulate and solve dynamic optimal control problems using a Pyomo.DAE framework and to investigate the influence of incorporating bifurcation-related information into the control formulation. By comparing conventional and bifurcation-aware control strategies, the study evaluates how nonlinear stability characteristics influence optimal system trajectories and overall control performance.

The novelty of this work lies in the integration of continuation-based bifurcation analysis, machine-learning-based regime identification, phase-space validation, and optimal control within a single computational framework. Rather than treating these techniques independently, the proposed methodology establishes a coherent workflow that links nonlinear system analysis with data-driven decision making and control design, making it readily applicable to a broad class of nonlinear engineering systems. The paper is organized as follows. The

model equations are first described, followed by the numerical procedures, results, discussion, and conclusions.

4. Mathematical Model and Governing Equations

The system considered in this work is a continuously stirred tank reactor (CSTR) in which an irreversible, exothermic, first-order reaction takes place. The reactor dynamics are described by coupled nonlinear ordinary differential equations that represent species and energy balances. Due to the strong temperature dependence of the reaction rate, the system exhibits nonlinear behavior, including multiple steady states and Hopf bifurcation-induced oscillations.

The model is derived under the standard assumptions of perfect mixing, constant density, constant heat capacity, and spatially uniform temperature and concentration inside the reactor. The dynamic evolution of the reactant concentration $C_A(t)$ is governed by a total mass balance on species A . The general form of the component balance in a CSTR is:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - r_A \quad (1)$$

Where C_A is the concentration of the reactant A inside the reactor, C_{A0} is the inlet concentration, F is the volumetric flow rate, V is the reactor volume, r_A is the reaction rate of species A .

For a first-order irreversible reaction, the rate law is given by:

$$r_A = k(T)C_A \quad (2)$$

where the temperature-dependent rate constant follows the Arrhenius expression:

$$k(T) = k_0 \exp\left(-\frac{E}{RT}\right) \quad (3)$$

Here, K_0 is the pre-exponential factor, E is the activation energy, R is the universal gas constant, and T is the reactor temperature. Substituting the reaction rate into the mass balance yields:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 \exp\left(-\frac{E}{RT}\right)C_A \quad (4)$$

This equation captures two competing mechanisms which are the convective inflow/outflow driving the concentration toward C_{A0} , and nonlinear consumption due to the temperature-dependent reaction rate. The energy balance describes the evolution of reactor temperature $T(t)$. It accounts for convective heat exchange, exothermic reaction heat release, and external heat removal via cooling. The general energy balance for a CSTR is:

$$\rho C_p \frac{dT}{dt} = \frac{F}{V} \rho C_p (T_0 - T) + (-\Delta H_r) r_A + \frac{UA}{V} (T_c - T) \quad (5)$$

Dividing through by ρC_p gives:

$$\frac{dT}{dt} = \frac{F}{V} (T_0 - T) + \frac{-\Delta H_r}{\rho C_p} r_A + \frac{UA}{\rho C_p V} (T_c - T) \quad (6)$$

Substituting the Arrhenius reaction rate:

$$\frac{dT}{dt} = \frac{F}{V} (T_0 - T) + \frac{-\Delta H_r}{\rho C_p} k_0 \exp\left(-\frac{E}{RT}\right)C_A + \frac{UA}{\rho C_p V} (T_c - T) \quad (7)$$

Where T_0 is the inlet feed temperature, T_c is the coolant/jacket temperature (control input), $\Delta H_r < 0$ for an exothermic reaction, and UA is the overall heat transfer coefficient times heat exchange area. Each term in the governing equations has a clear physical interpretation. The Convective terms $\frac{F}{V}(C_{A0} - C_A)$, $\frac{F}{V}(T_0 - T)$ represent inflow–outflow exchange. They act as linear stabilizing terms, driving the system toward inlet conditions.

The Reaction nonlinearity comes from $k_0 \exp(-\frac{E}{RT})C_A$. This term introduces strong nonlinearity due to the exponential dependence on temperature. As temperature increases, reaction rate increases sharply, creating positive feedback between temperature and reaction rate. This feedback mechanism is the primary source of multiplicity of steady states, instability, and Hopf bifurcation behavior.

The Heat generation term is $\frac{-\Delta H_r}{\rho C_p} k C_A$. For exothermic reactions (), this term acts as a heat source, further increasing temperature and reinforcing thermal runaway tendencies. The Heat removal term represents cooling through a jacket or external heat exchanger. It provides a stabilizing mechanism that counteracts thermal instability.

The balance between heat generation (reaction), and heat removal (cooling), determines whether the system settles to a steady state or exhibits oscillations. The coupling between C_A and T creates a strongly nonlinear dynamical system. The exponential temperature dependence of the reaction rate introduces feedback that can destabilize steady states.

As the bifurcation parameter T_0 is varied, the system may exhibit a single stable steady state, multiple steady states, and/or oscillatory limit cycles via Hopf bifurcation. In particular, Hopf bifurcation occurs when a pair of complex conjugate eigenvalues of the Jacobian crosses the imaginary axis, leading to the emergence of periodic oscillations.

This transition is central to the nonlinear behavior studied in this work and motivates both the data-driven classification and optimal control formulation. The resulting model is a two-state nonlinear dynamical system:

$$\begin{aligned}\frac{dC_A}{dt} &= \frac{F}{V}(C_{A0} - C_A) - k_0 e^{-E/(RT)} C_A \\ \frac{dT}{dt} &= \frac{F}{V}(T_0 - T) + \frac{-\Delta H_r}{\rho C_p} k_0 e^{-E/(RT)} C_A + \frac{UA}{\rho C_p V}(T_c - T)\end{aligned}\quad (8)$$

Despite its compact form, the system exhibits rich nonlinear dynamics including bifurcation and oscillations, making it an ideal benchmark for studying data-driven regime classification and optimal control near instability boundaries.

5. Numerical Method

5.1. Bifurcation Analysis

Continuation and bifurcation computations were carried out using the MATLAB-based software MATCONT. Bifurcation analysis provides important insights into the mechanisms underlying the existence of multiple steady states and self-sustained oscillations in nonlinear dynamical systems. In particular, branch points and limit points are associated with the emergence of multiple steady-state solutions, whereas oscillatory dynamics and periodic solutions originate from Hopf bifurcations. The package, originally developed and subsequently enhanced by several researchers, enables the systematic identification of limit points, branch points, and Hopf bifurcation points in nonlinear dynamical models [31].

5.2. Data-Driven Characterization of Nonlinear Dynamics

To complement the bifurcation analysis and provide a systematic link between parameter variations and qualitative system behavior, a data-driven framework was developed in the vicinity of the critical bifurcation region. A set of simulations was performed by varying the primary bifurcation parameter over a prescribed range surrounding the identified Hopf point. For each parameter value, the corresponding temporal response of the dynamical system was computed after transient removal to ensure that only asymptotic behavior was retained.

From the resulting trajectories, a set of statistical features was extracted to construct a reduced-order representation of the system dynamics. These features typically include measures of central tendency, dispersion, and amplitude, which collectively capture essential characteristics of steady-state and oscillatory regimes. The resulting dataset provides a compact mapping between the bifurcation parameter and the qualitative nature of the system response.

5.3. Machine Learning-Based Regime Classification

Based on the constructed dataset, a supervised learning framework was employed to classify the system behavior into distinct dynamical regimes. In particular, the objective of the classifier is to distinguish between steady-state and oscillatory solutions using only feature-level information derived from time-domain simulations. This approach enables rapid identification of regime transitions without requiring repeated numerical integration of the governing equations.

The classification boundary implicitly captures the transition between stable equilibrium behavior and sustained oscillations induced by the Hopf bifurcation. As such, the trained model serves as a surrogate representation of the nonlinear stability landscape in the vicinity of the critical parameter region.

5.4. Phase Space Analysis

To further validate the identified dynamical regimes, phase space reconstruction was performed using the relevant state variables of the system. The resulting phase portraits provide a geometric interpretation of the system dynamics, where stable equilibria appear as fixed points and oscillatory behavior manifests as closed periodic orbits. In particular, the presence of a limit cycle confirms the existence of sustained oscillations associated with the Hopf bifurcation, while convergence to a fixed point indicates stable steady-state behavior.

This phase-space representation provides an additional qualitative verification of the regime classification obtained from the data-driven approach, ensuring consistency between numerical simulations and geometric system behavior.

6. Link to Optimal Control Formulation

The insights obtained from bifurcation analysis, data-driven classification, and phase-space characterization are subsequently used to motivate the optimal control formulation. In particular, the presence of oscillatory regimes near the bifurcation point necessitates the design of control strategies that stabilize the system and mitigate undesirable dynamics. This motivates the development of both baseline and bifurcation-aware optimal control formulations, which are presented in the following section.

6.1. Optimal Control

The optimal control problem is formulated within Pyomo.DAE framework. In this approach, the continuous-time dynamic system is formulated as a nonlinear programming (NLP) problem via discretization methods such as orthogonal collocation, enabling numerical solution with standard NLP solvers. The resulting NLP is solved using IPOPT (Wächter and Biegler, 2006), which efficiently handles large-scale constrained nonlinear optimization problems [32].

7. Results

When Bifurcation Analysis was performed with MATCONT, a Hopf bifurcation Point with a first Lyapunov coefficient of 1.188512×10^{-2} was found at (C_A, T, T_0) values of (0.398963 270.644316 110.294393), additionally a limit point was also located at (C_A, T, T_0) values of (0.414461 269.061585 110.254634). The bifurcation diagram and the limit cycle caused by the Hopf bifurcation are shown in Figs 1a and 1b.

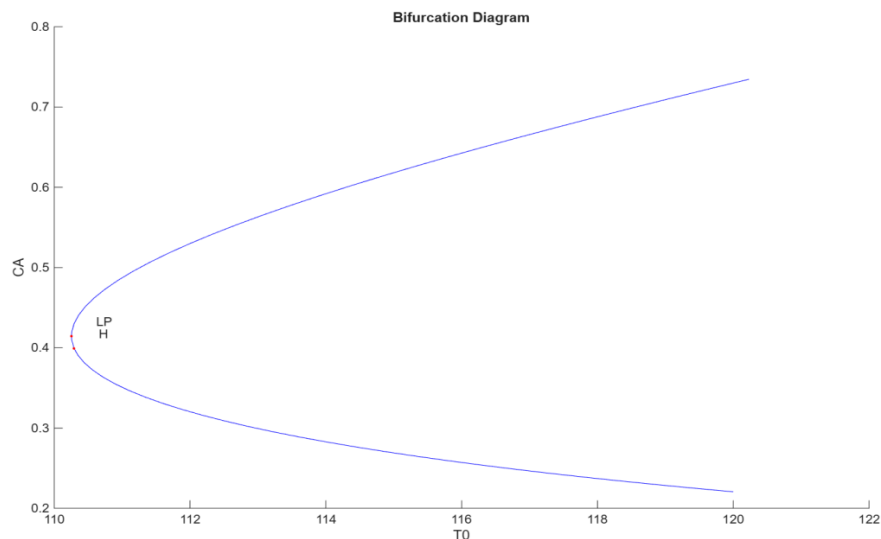


Figure 1a: Bifurcation Diagram

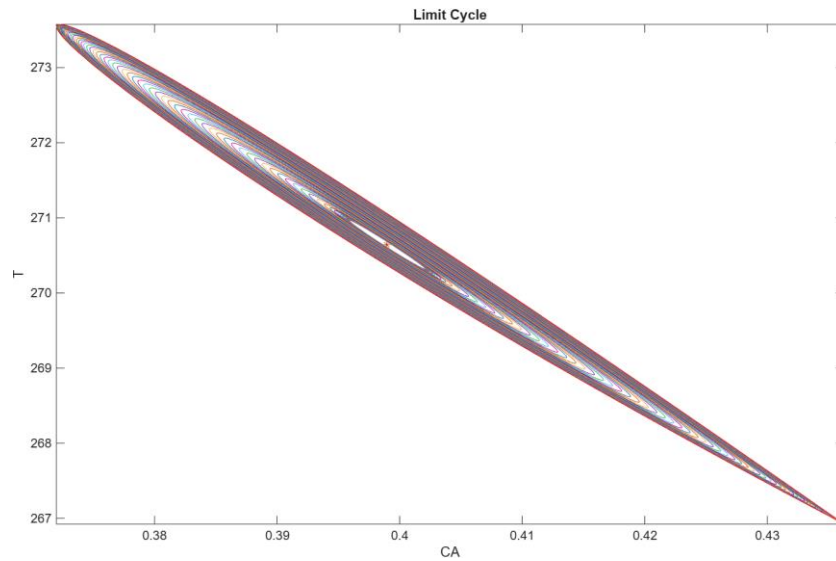


Figure 1b: Limit Cycle

For the optimal control, the objective function $\sum (T(t) - 300)^2 + 0.1 * (T_c(t) - 276)^2$ is minimized without (the objective function value was 900) and with Hopf awareness (the objective function value was 900.14). Although the two solutions are very close to each other the dynamic profiles obtained in both the cases were different.

The phase portrait in Fig. 4 highlights the presence of a stable limit cycle in the uncontrolled system, confirming the onset of self-sustained oscillations near the Hopf bifurcation. This motivates the development of the optimal control strategies presented in the next section, where control action is designed to stabilize the system and reduce oscillatory behavior in the vicinity of the bifurcation region.

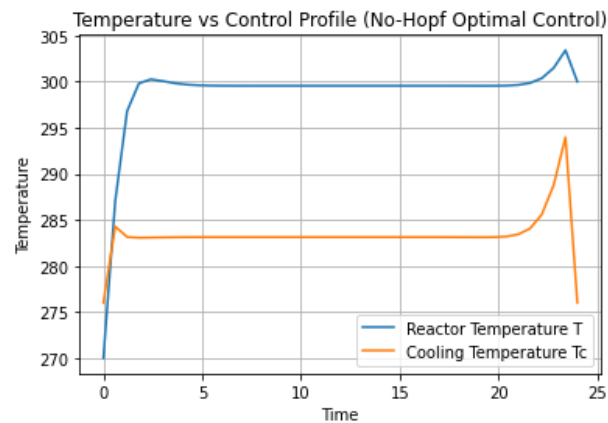


Figure 2a: Optimal Control Temperature Profile without Hopf Awareness

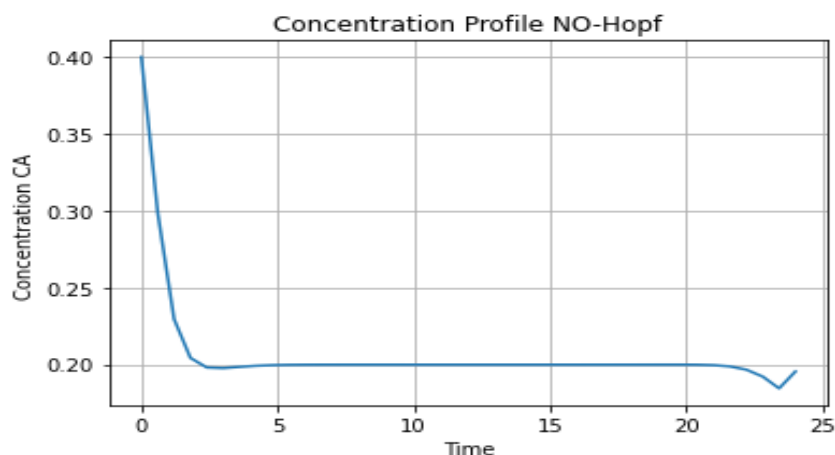


Figure 2b: Optimal Control Concentration Profile without Hopf Awareness

8. Discussion of Results

The results obtained from the bifurcation analysis, phase space reconstruction, and optimal control studies provide a comprehensive understanding of the nonlinear behavior of the system in the vicinity of the Hopf bifurcation point. The combination of continuation methods and dynamic simulation reveals a rich structure of steady-state multiplicity and oscillatory dynamics, which plays a central role in the observed system behavior.

The bifurcation analysis performed using MATCONT identified a Hopf bifurcation point at $(0.398963, 270.644316, 110.294393)$, with a corresponding first Lyapunov coefficient of 1.188512×10^{-2} .

The positive sign of the Lyapunov coefficient indicates that the Hopf bifurcation is supercritical in nature, leading to the emergence of a stable limit cycle beyond the critical parameter value.

This implies that the oscillatory solutions generated in the vicinity of the bifurcation point are dynamically stable and persist over time, rather than diverging or decaying. In addition, a limit point was detected at $(0.414461, 269.061585, 110.254634)$, indicating the presence of a turning point in the steady-state branch, which is often associated with saddle-node type behavior and contributes to multistability in the system.

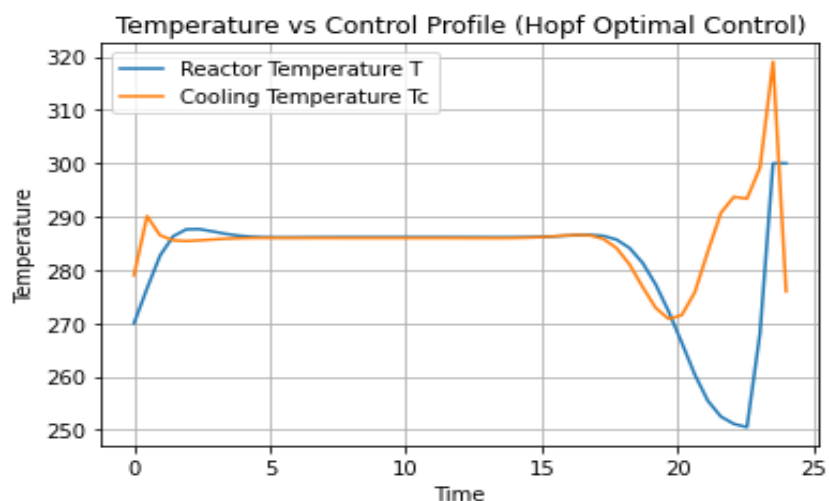


Figure 3a: Optimal Control Temperature Profile with Hopf Awareness

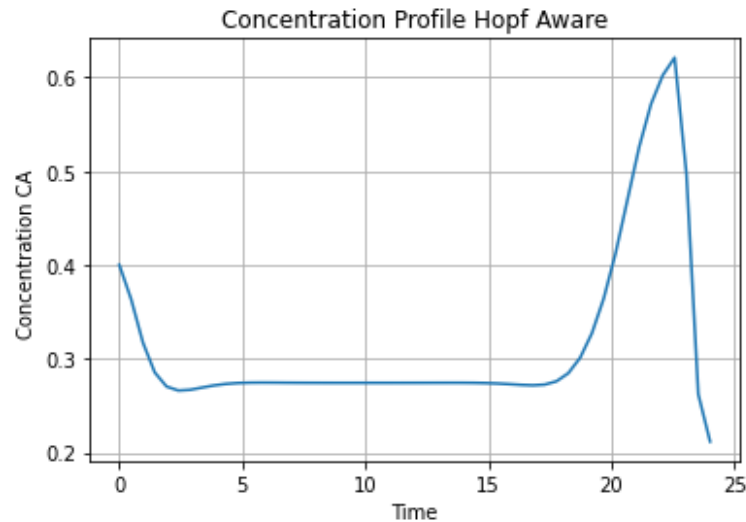


Figure 3b: Optimal Control Concentration Profile with Hopf Awareness

The bifurcation diagram and the corresponding limit cycle, shown in Figs. 1 and 1b, clearly illustrate the transition from steady-state behavior to sustained oscillations.

As the bifurcation parameter is varied, the system loses stability at the Hopf point and transitions into a periodic orbit. The emergence of this limit cycle confirms the nonlinear nature of the system and highlights the sensitivity of the dynamics to parameter variations in the vicinity of critical operating conditions. Further insight into the system dynamics is provided by the phase portrait shown in Fig. 4. The phase plane representation reveals a closed trajectory in the state space, confirming the existence of a stable limit cycle predicted by the bifurcation analysis. This closed orbit indicates that the system does not converge to a fixed equilibrium but instead evolves toward sustained oscillations in both state variables.

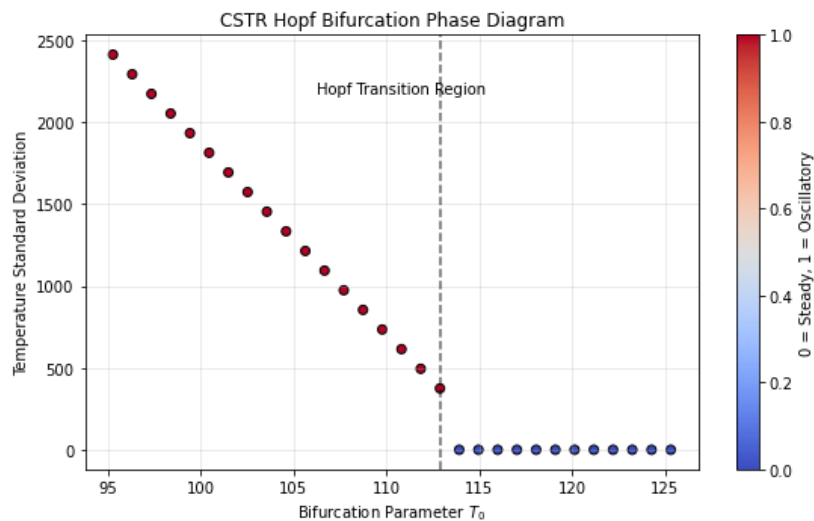


Figure 4: Phase Diagram

The phase portrait therefore provides a geometric interpretation of the oscillatory regime and serves as an important validation of the numerical continuation results obtained from MATCONT. The agreement between bifurcation analysis and phase space behavior strengthens the conclusion that the system exhibits robust oscillatory dynamics near the Hopf bifurcation.

The presence of such oscillatory behavior has direct implications for process operation and control. In practical systems, sustained oscillations may lead to undesirable fluctuations in key process variables, reduced product quality, and increased operational instability. This motivates the development of control strategies capable of stabilizing the system and suppressing oscillations in the critical

operating region.

To address this, optimal control formulations were implemented and solved using a discretized nonlinear programming approach. Two cases were considered: a baseline optimal control problem without explicit bifurcation awareness and a modified formulation incorporating bifurcation-related insights.

The objective function values obtained in both cases are very close, with values of approximately 900 for the baseline case and 900.14 for the bifurcation-aware formulation. The small difference in objective values suggests that both controllers achieve similar levels of performance in terms of the defined cost function.

However, despite the similarity in objective values, the resulting dynamic trajectories exhibit noticeable differences. This indicates that the inclusion of bifurcation-related information influences the structure of the optimal solution, even if it does not significantly alter the scalar objective value. In nonlinear dynamical systems, such behavior is common, as multiple control trajectories may yield comparable cost values while producing distinct transient and steady-state dynamics. This highlights the importance of analyzing not only the objective function but also the qualitative behavior of the system trajectories when evaluating control performance.

The phase portrait and bifurcation results together provide a clear explanation for this behavior. Since the uncontrolled system exhibits a stable limit cycle near the Hopf bifurcation, the control action must compete with inherent nonlinear oscillatory tendencies. As a result, even small modifications in the control formulation can lead to different trajectory structures, particularly in the transient regime and near the oscillatory manifold.

Overall, the results demonstrate a strong coupling between nonlinear dynamics and control performance. The bifurcation analysis identifies the critical regions where qualitative changes in system behavior occur, while the phase portrait confirms the existence of stable oscillations. The optimal control analysis shows that although performance metrics may remain similar across formulations, the underlying dynamic behavior can differ significantly depending on whether bifurcation information is incorporated into the control design.

These findings emphasize the importance of integrating nonlinear dynamical analysis with control optimization. In particular, bifurcation-aware control design provides additional insight into system behavior in regions where classical optimal control formulations may not fully capture the complexity of the underlying dynamics. This integrated approach is essential for reliable operation and control of nonlinear systems operating near instability boundaries such as Hopf bifurcations.

This work demonstrates a systematic integration of bifurcation analysis, data-driven classification, and optimal control for nonlinear dynamical systems operating near critical instability boundaries.

By identifying Hopf bifurcation points and associated limit cycles, the study provides a clear understanding of the transition from steady-state to oscillatory behavior.

The development of a feature-based dataset enables efficient characterization of system regimes without repeated numerical simulations. Machine learning-based classification offers a fast surrogate tool for detecting dynamic transitions in parameter space. Phase space analysis further validates the presence of stable limit cycles and strengthens the physical interpretation of the nonlinear dynamics.

The optimal control framework shows how system behavior can be regulated even in the presence of inherent oscillatory tendencies. Although objective function values remain similar, significant differences in dynamic trajectories highlight the sensitivity of nonlinear control solutions.

The proposed bifurcation-aware perspective enhances traditional control design by incorporating stability structure information. This approach is general and can be extended to other nonlinear chemical and physical systems exhibiting bifurcations. Overall, the study provides a unified framework linking nonlinear dynamics, data science, and optimal control for improved system understanding and regulation.

9. Conclusions

This study presented an integrated computational framework for the analysis and control of nonlinear dynamical systems operating in the vicinity of critical bifurcation points. Numerical continuation using MATCONT was employed to identify the principal bifurcation structures governing the system dynamics, including the location of the Hopf bifurcation and the associated limit point.

The bifurcation analysis demonstrated the transition from stable steady-state operation to sustained oscillatory behavior, while the

computed first Lyapunov coefficient confirmed the nature of the Hopf bifurcation. These results provided a comprehensive understanding of the nonlinear stability characteristics of the system and established the critical operating region for subsequent analysis.

A data-driven methodology was then developed to characterize the dynamic behavior around the bifurcation point. By generating simulation data over the critical parameter range and extracting representative statistical features, a supervised machine learning classifier was constructed to distinguish between steady-state and oscillatory operating regimes.

The resulting classifier demonstrated that qualitative system behavior can be accurately identified using feature-based information, providing a computationally efficient alternative to repeated numerical simulations.

Phase space analysis further validated the classification results by clearly illustrating the existence of stable limit cycles associated with the oscillatory regime.

Dynamic optimal control problems were subsequently formulated within the Pyomo.DAE framework and solved using IPOPT. Both a conventional optimal control formulation and a bifurcation-aware formulation were investigated.

Although the objective function values obtained from the two formulations were very similar, the resulting dynamic trajectories exhibited noticeable differences, demonstrating that incorporating nonlinear stability information can influence the structure of the optimal solution even when overall performance metrics remain comparable.

This observation highlights the importance of considering the underlying nonlinear dynamics during control system design rather than relying solely on objective function values. Overall, the proposed methodology establishes a unified framework that combines bifurcation analysis, machine learning, phase space analysis, and optimal control into a coherent workflow for studying nonlinear systems.

The approach is sufficiently general to be applied to a wide range of engineering applications exhibiting nonlinear instabilities, including chemical reactors, environmental processes, biochemical systems, and energy systems. Future work will focus on extending the methodology to higher-dimensional systems, incorporating advanced machine learning algorithms, and developing real-time bifurcation-aware predictive control strategies for complex nonlinear processes.

Data Availability Statement

All data used is presented in the paper.

Conflict of Interest

The author, Dr. Lakshmi N Sridhar has no conflict of interest.

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