Reconstructing transitions between dynamical regimes driven by unknown variables using universal normal forms

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Abstract

Problem

Several model architectures can be proposed for a given biological system. Each model has a vast parameter space, with hidden control variables influencing the system. Dynamical shifts are challenging to model, and real-world scenarios often involve complex dynamical regimes.

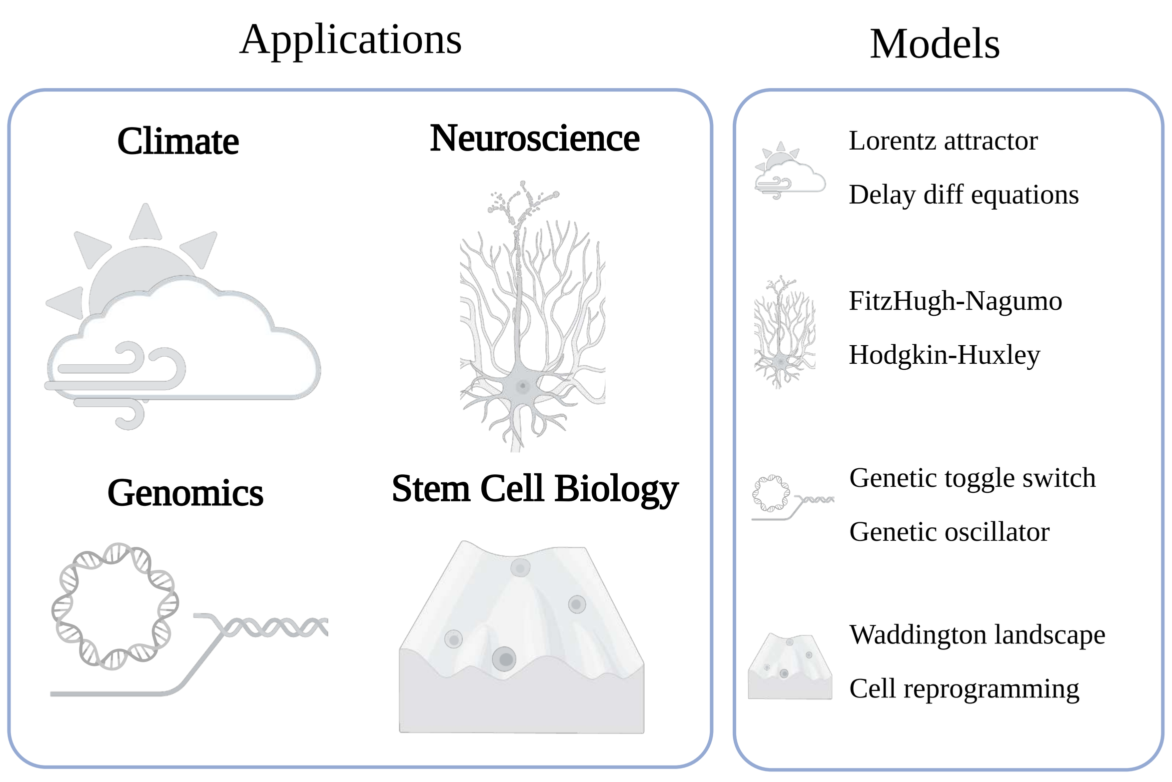
Our IHCV Method

Our method uses normal forms as universal, scalable, and minimal dynamical building blocks. It formalizes the notion of hidden variables and outperforms state-of-the-art methods for model discovery under real-world assumptions.

Results

We successfully uncover the underlying equations and unobserved hidden variables in data generated from the toggle switch, genetic oscillator, Waddington landscape, and 11 other models. The predicted models can reproduce dynamical regimes not included in the training data, without requiring access to derivatives or large datasets.

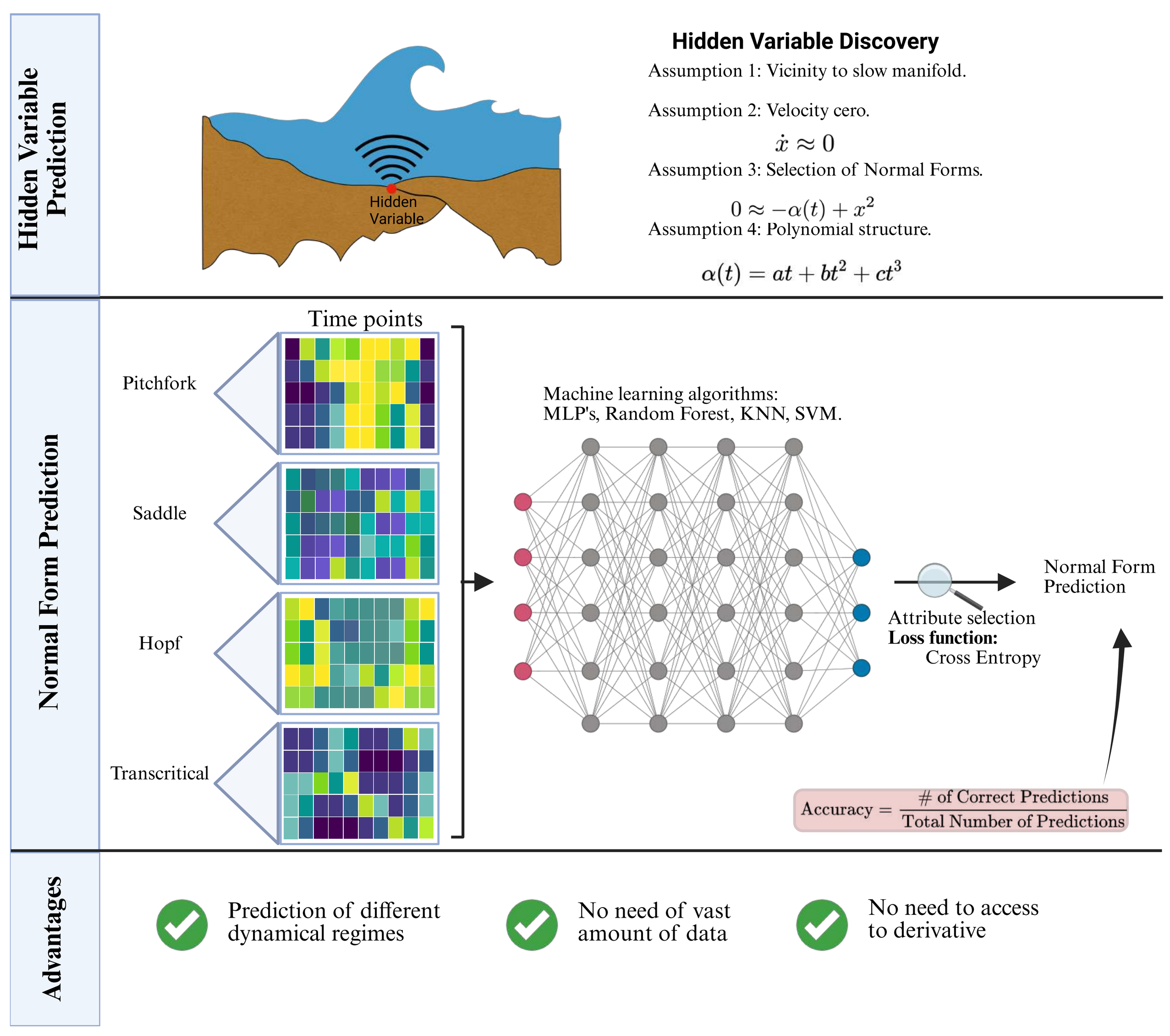
Current Challenges



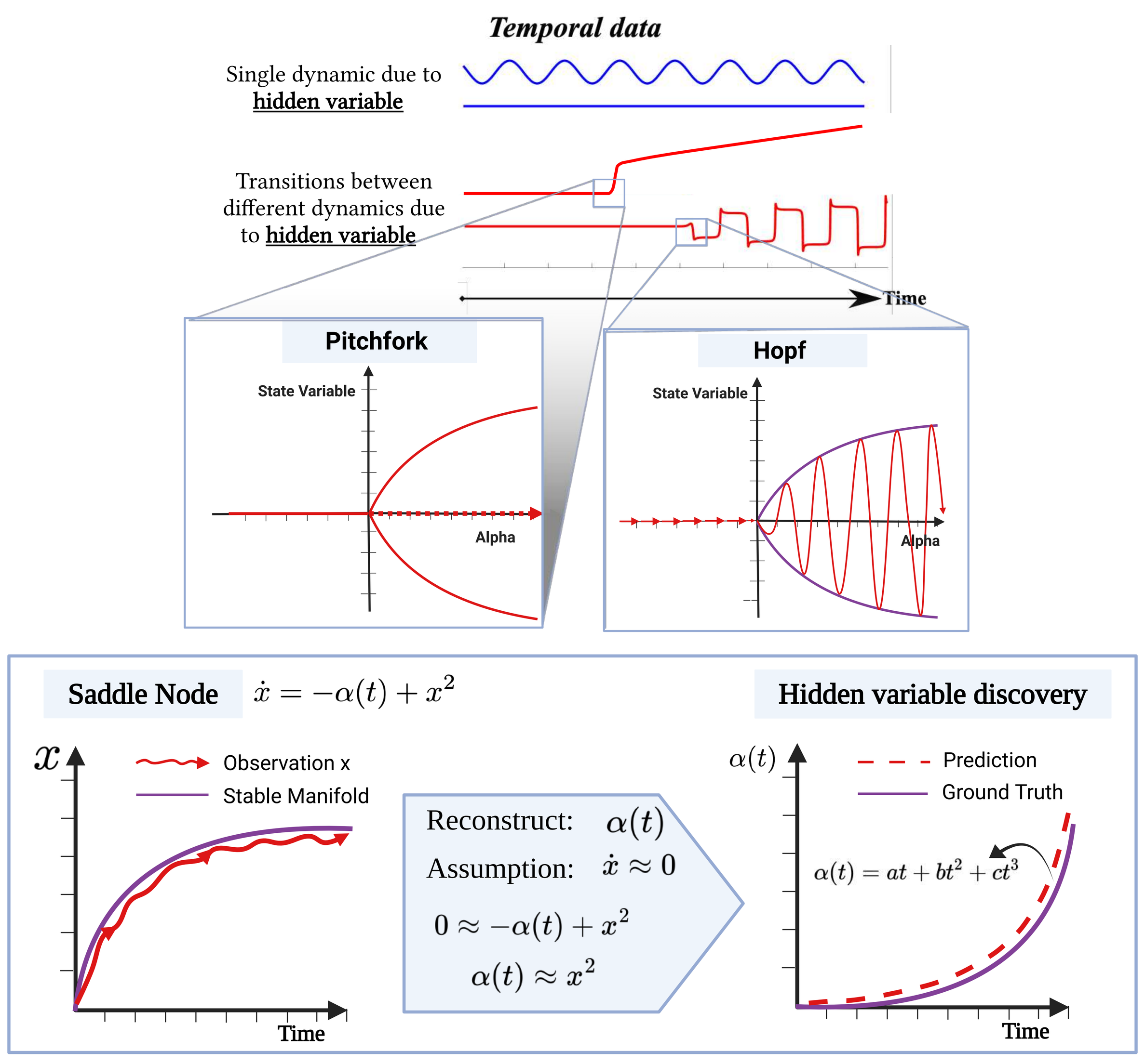
Current challenges:

- Lack of access to fundamental equations.
- Nature does not provide extensive data.
- Cannot measure all the variables.
- Unreal assumptions.
- Current predicted models are unstable (stiffness).

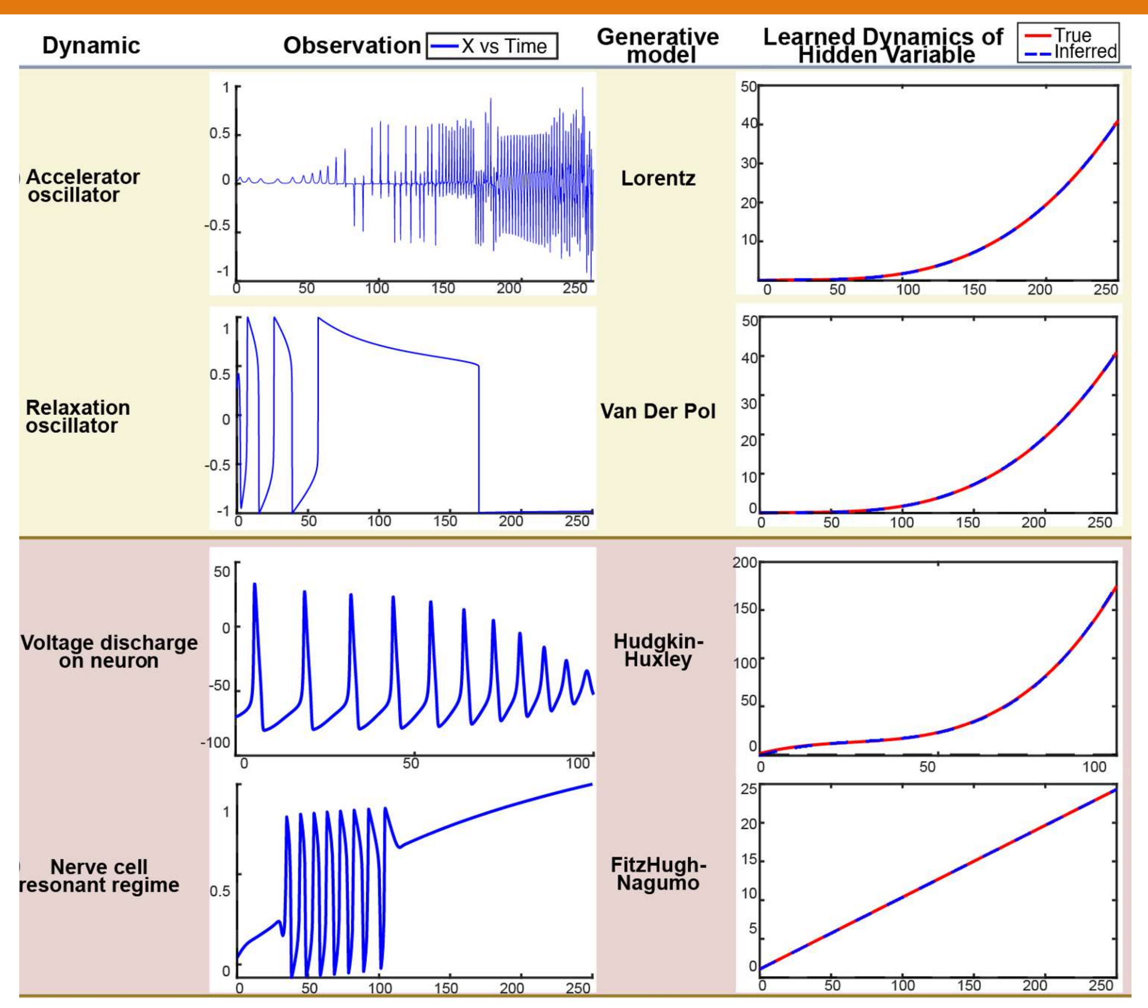
General Overview



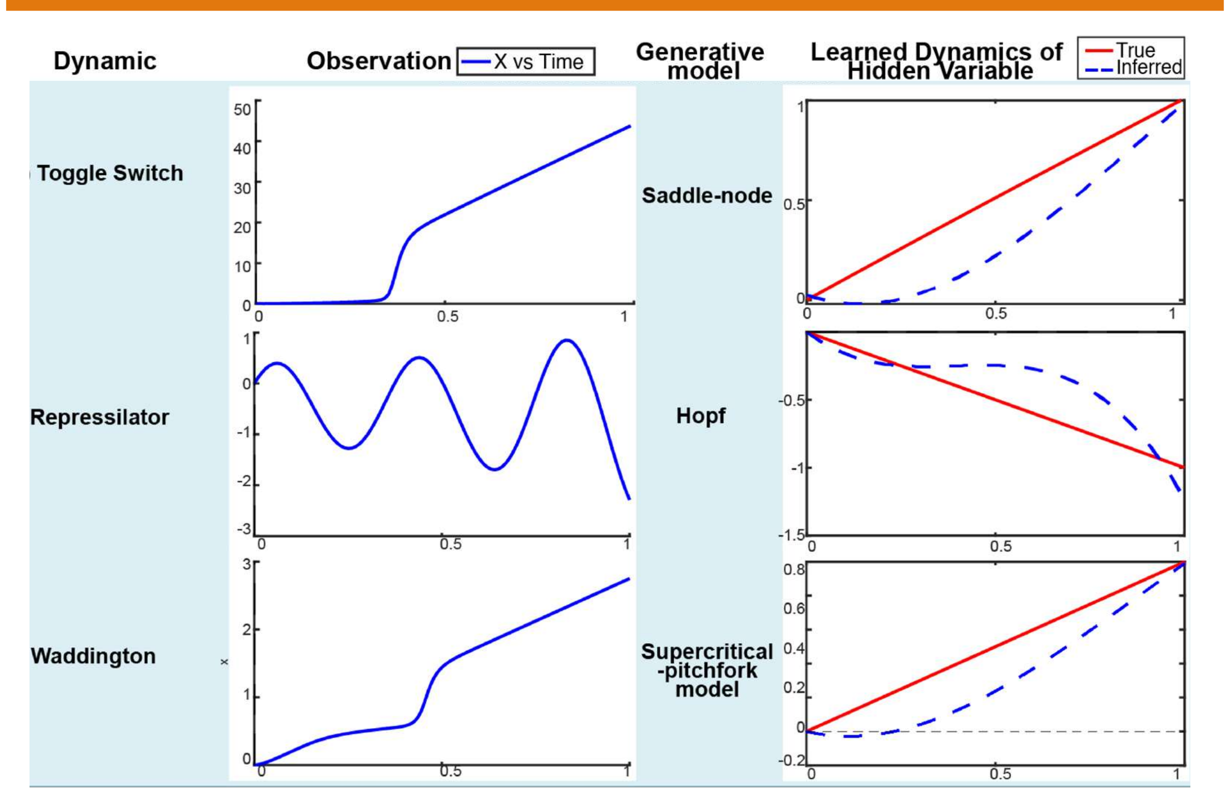
Formalizing the Notion of Hidden Variables



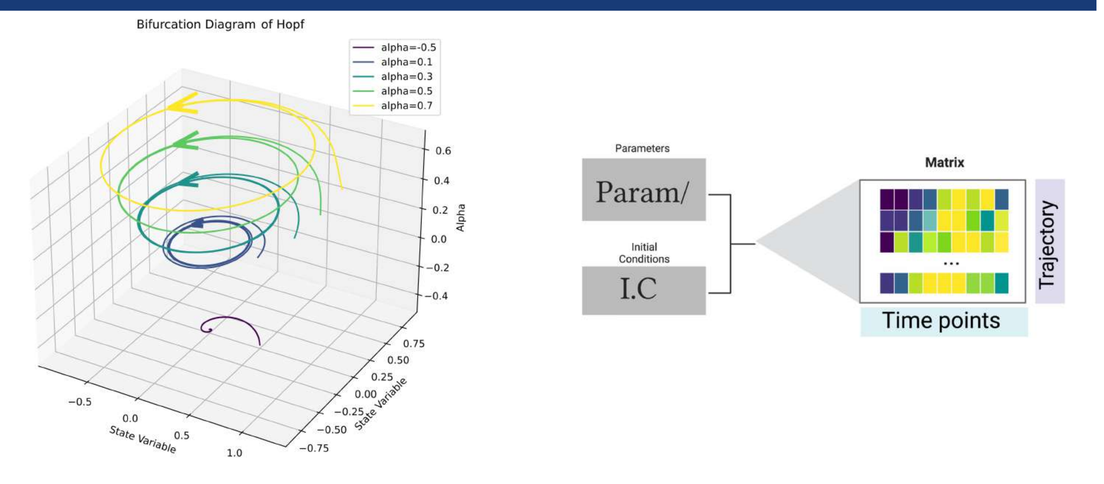
VALIDATION



DISCOVERY FOR UNKNOWN SYSTEMS



Normal Form Selection for Unknown Equations



Saddle Node-Pitchfork Hybrid System:

$$
\begin{aligned}
x' &= r_1 + x^2 + w_{yx}y && \text{(Saddle Node)} \\
y' &= r_2 y - y^3 + w_{xy}x && \text{(Pitchfork)}
\end{aligned} \tag{5}
$$

Saddle Node-Hopf Hybrid System:

$$
\begin{aligned}
x' &= r_1 + x^2 + W && \text{(Saddle Node)} \\
\dot{y} &= \mu y - z - y(y^2 + z^2) + W && \text{(Hopf)} \\
\dot{z} &= y + \mu z - z(y^2 + z^2) + W && \text{(Hopf)}
\end{aligned} \tag{6}
$$

Saddle Node-Transcritical Hybrid System:

$$
\begin{aligned}
x' &= r_1 + x^2 + W && \text{(Saddle Node)} \\
y' &= r_2 y - y^2 + W && \text{(Transcritical)}
\end{aligned} \tag{7}
$$

Pitchfork-Hopf Hybrid System:

$$
\begin{aligned}
x' &= r_1 x - x^3 + W && \text{(Pitchfork)} \\
\dot{y} &= \mu y - z - y(y^2 + z^2) + W && \text{(Hopf)} \\
\dot{z} &= y + \mu z - z(y^2 + z^2) + W && \text{(Hopf)}
\end{aligned} \tag{8}
$$

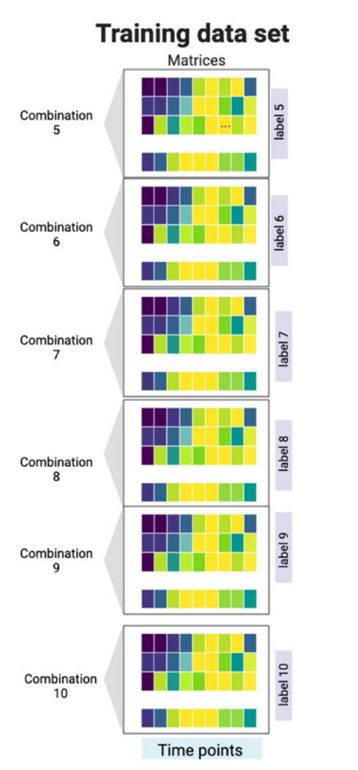
Pitchfork-Transcritical Hybrid System:

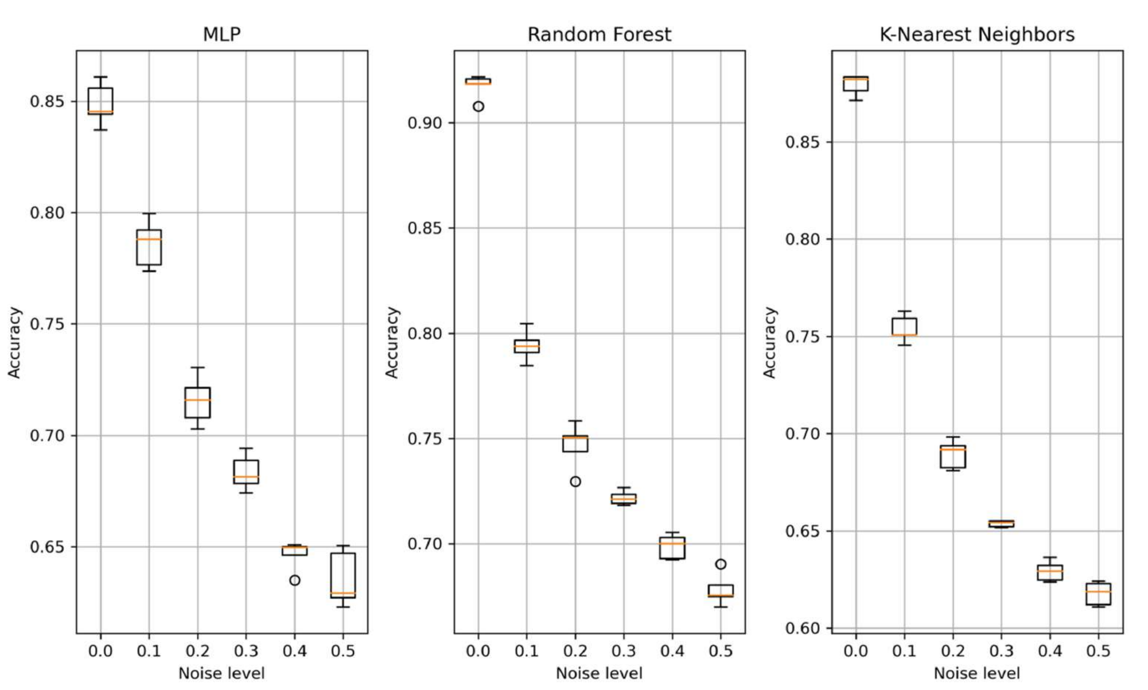
$$
\begin{aligned}
x' &= r_1 x - x^3 + W && \text{(Pitchfork)} \\
y' &= r_2 y - y^2 + W && \text{(Transcritical)}
\end{aligned} \tag{9}
$$

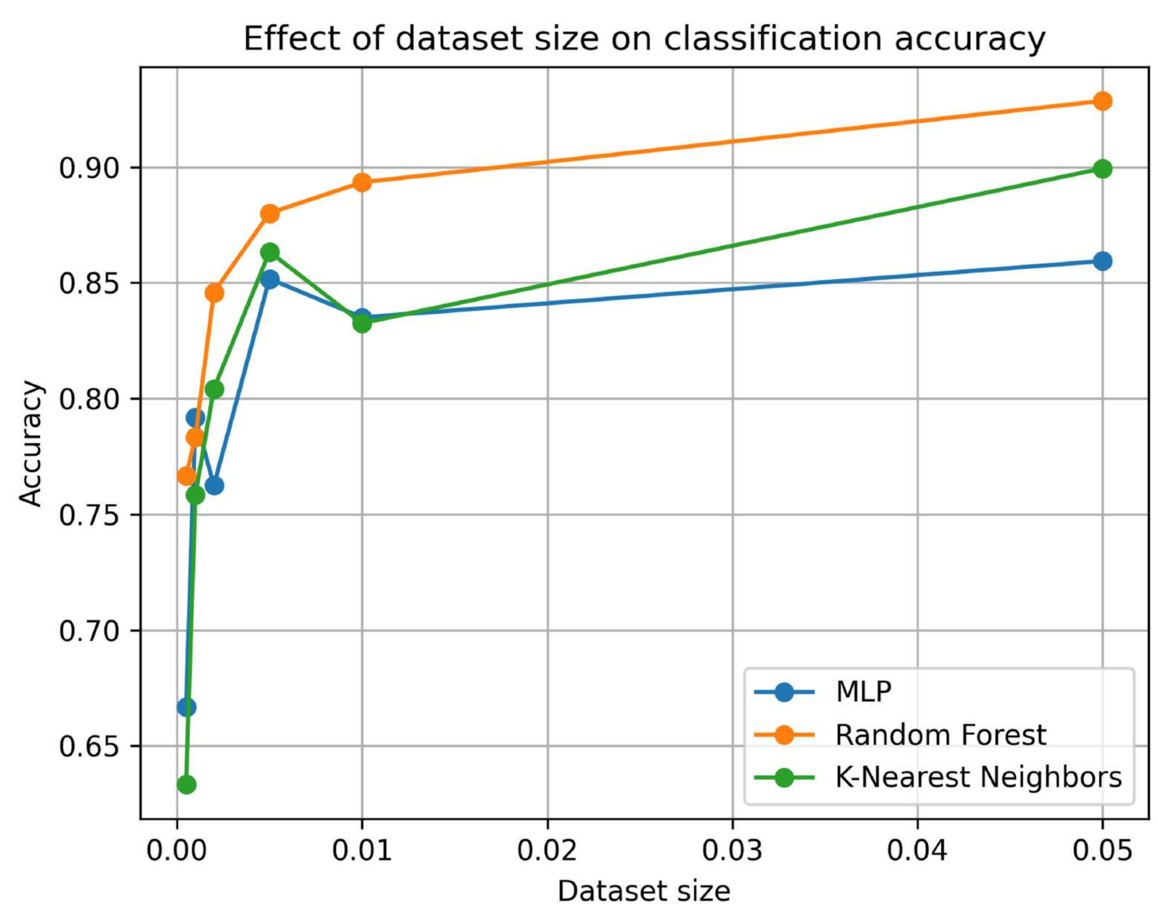
Hopf-Transcritical Hybrid System:

$$
\begin{aligned}
\dot{x} &= \mu x - y - x(x^2 + y^2) + W && \text{(Hopf)} \\
\dot{y} &= x + \mu y - y(x^2 + y^2) + W && \text{(Hopf)} \\
z' &= r_2 z - z^2 + W && \text{(Transcritical)}
\end{aligned} \tag{10}
$$

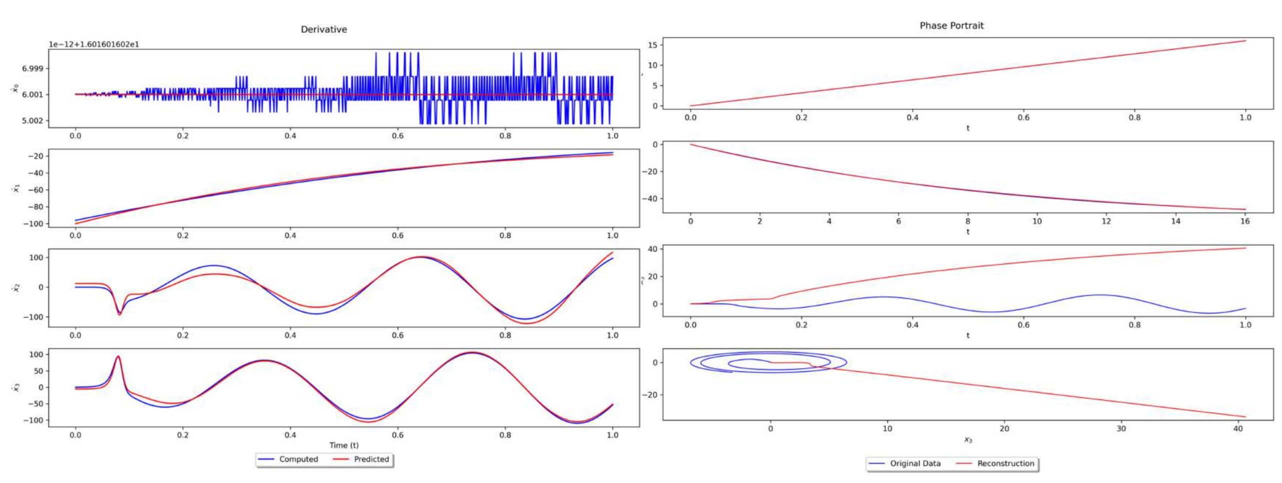
Training data set







Comparison with Current Techniques

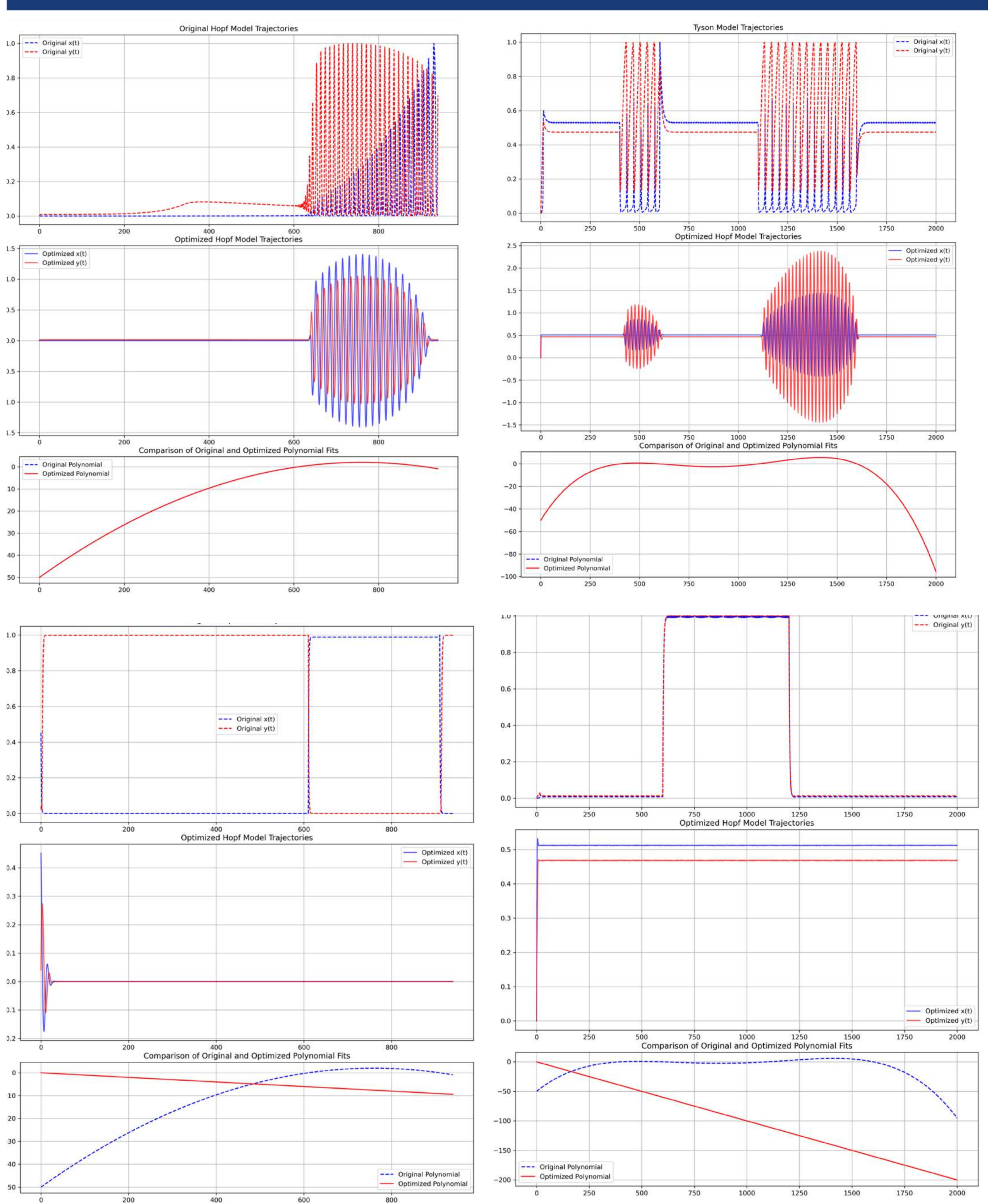


$x_0 = time'$
$x_1' = \alpha'$
$x_2' = Hopf_1$
$x_3' = Hopf_2$

IHCV		
1 Trajectory (T)		
R^2 Deriv	R^2 State	MSE
0.72363	0.9954	0.17042

Library Size	SINDY											
	1 T			4 T			6 T			16 T		
	R^2 Deriv	R^2 State	Stiff-Ratio	R^2 Deriv	R^2 State	Stiff-Ratio	R^2 Deriv	R^2 State	Stiff-Ratio	R^2 Deriv	R^2 State	Stiff-Ratio
0	0.02	0.16	1.00	0.00	0.30	1.00	0.01	0.40	1.00	0.01	0.35	1.00
1	0.76	0.79	317.10	0.41	0.37	238.35	0.33	0.54	399.18	0.31	0.58	416.23
2	0.77	-	3.3E+05	0.45	0.05	245.81	0.38	0.05	369.60	0.38	0.03	465.00
3	0.77	-0.84	9389.80	0.71	-5.81	192.56	0.69	0.49	338.21	0.67	0.25	425.21
4	0.77	0.23	13715.28	0.74	-	31.41	0.72	-	60.49	0.68	-	447.84
5	0.75	-20.23	381.45	0.75	-	95.47	0.74	-	26.82	0.71	-0.08	402.31
6	0.28	0.44	23473.88	0.74	-	3924.49	0.75	-118.55	38.76	0.71	-	410.84
7	0.28	0.44	23473.88	0.65	-0.09	173.56	0.72	0.26	396.53	0.71	-	402.43
8	0.28	0.44	23252.23	0.23	-	Inf	0.34	0.12	388.81	0.70	-1.02	402.82
9	0.51	-	Inf	0.37	-0.50	443.52	0.31	0.48	364.97	0.63	-0.53	431.73
10	-2.5E+26	-	NaN	0.12	-	Inf	0.13	-	Inf	0.11	-	Inf
11	-2.5E+26	-	NaN	-3.1E+25	-	NaN	-3.7E+25	-	Inf	-4.6E+25	-	Inf
12	-2.5E+26	-	NaN	-3.1E+25	-	NaN	-3.7E+25	-	NaN	-4.6E+25	-	NaN
13	-2.5E+26	-	NaN	-3.1E+25	-	NaN	-3.7E+25	-	NaN	-4.6E+25	-	NaN
14	-2.5E+26	-	NaN	-3.1E+25	-	NaN	-3.7E+25	-	NaN	-4.6E+25	-	NaN
15	-2.5E+26	-	NaN	-3.1E+25	-	NaN	-3.7E+25	-	NaN	-4.6E+25	-	NaN

Learning New Dynamical Regimes



Future Research

We aim to capture complex transitions and dynamical shifts in intricate systems. Building on our current work with two normal form combinations (e.g., Saddle-Hopf, Saddle-Pitchfork), we plan to expand to 4–6 combinations, constructing a comprehensive library of normal forms to model these systems more effectively. Such dynamics remain underexplored in high-dimensional data applications. Thus, we will address scalability by extending IHCV to higher-dimensional systems.

References

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