Automated discovery of fundamental variables hidden in experimental data

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1 Introduction

1.1 Goal

1. To explicitly find identify the intrinsic dimension of a system and the hidden state variable from visual information(raw camera).
2. Classical observation: $128 \times 128 \times 3$ pixels of RGB image, 49152 frames
3. Intrinsic Physics: Swinging Pendulum with two variable(angle and angular velocity)

1.2 Approach Sketch

Two-stage algorithm:

1. Training a predictive Neural Network with Encoder-Decoder structure
2. Calculate the intrinsic dimension (ID) of the latent embedding using Manifold learning
3. Training a latent reconstuction Neural Network to identify the governing state variable

Besides, the paper leverage the discovered neural state variables as both an intermediate representation and an evaluation metric for stable long-term future predictions of system behaviours.

2 Method

The dynamics of a physical system: provided the ambient space $\mathcal{X}$, state space $\mathcal{S} \subset \mathcal{X}$, the dynamical system is

$$X_{t+\mathrm{dt}} = F(X_t), t = 0, \ldots \mathrm{ndt}$$

where $X_t \in \mathcal{S}$ is the current state, $F: \mathcal{S} \rightarrow \mathcal{S}$ is the evolution.

2.1 Stage 1

Here $\mathcal{X}$ is a high dimensional image space, such as $128 \times 128 \times 3$ RGB channel. To train a predictive model, we use an Encoder network g_E and a Decoder network g_D, the input is X_t, the first output is $L_{t \to t+\mathrm{dt}} = g_E(X_t)$ is the embedding of next time instant, the output is $\hat{X}_{t+\mathrm{dt}} = g_D(L_{t \to t+\mathrm{dt}})$. We use a supervise learning paradigm

$$\mathcal{L} = \mathbb{E}_X[|| g_D(g_E(X_t)) - X_{t+\mathrm{dt}}||_2^2]$$

The learned mapping is $\hat{F} = g_D \circ g_E$ is a numerical approximation of F.

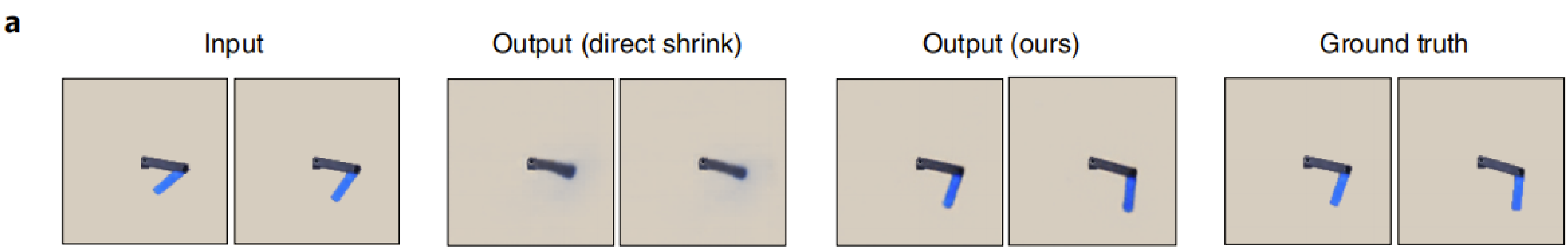


图 1. Unsatisfied prediction using Encoder-Decoder

The dimension LD of $L_{t \to t+\mathrm{dt}}$ is a parameter of learning.

2.2 ID estimation

ID is the topological dimension of the state space $\mathcal{S}$ as a manifold in the ambient space $\mathcal{X}$. The ID is independent of specific representations of the system.

Classical Approach: Using a Autoencoder Network and keep reducing the size of the latent embedding vector through trial and error until the output is no longer valid.

2.3 Levina-Bickel algorithm for ID estimation

A key geometric observation is that the number of data points within distance r from any given data point $L^{(i)}$ is proportional to r^{ID} where r is small

1. We collect the latent variable $\{L^{(1)}, \ldots, L^{(N)}\}$ by using the Encoder Network on N sample

2. The local ID estimator near $L^{(i)}$ is $\frac{1}{k-2} \sum_{j=1}^{k-1} \log \frac{T_k(L^{(i)})}{T_j(L^{(i)})}$ where $T_k(L^{(i)})$ is the Euclidean distance between $L^{(i)}$ and its k-th nearest neighbour in $\{L^{(1)}, \ldots,$ $L^{(N)}\}$.

3. The global estimator is

$$\mathrm{ID}_{L-B} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{k-2} \sum_{j=1}^{k-1} \log \frac{T_k(L^{(i)})}{T_j(L^{(i)})}$$

4. The estimated ID values are rounded to the nearest even integer, as position and velocity variables are in pairs in our systems.

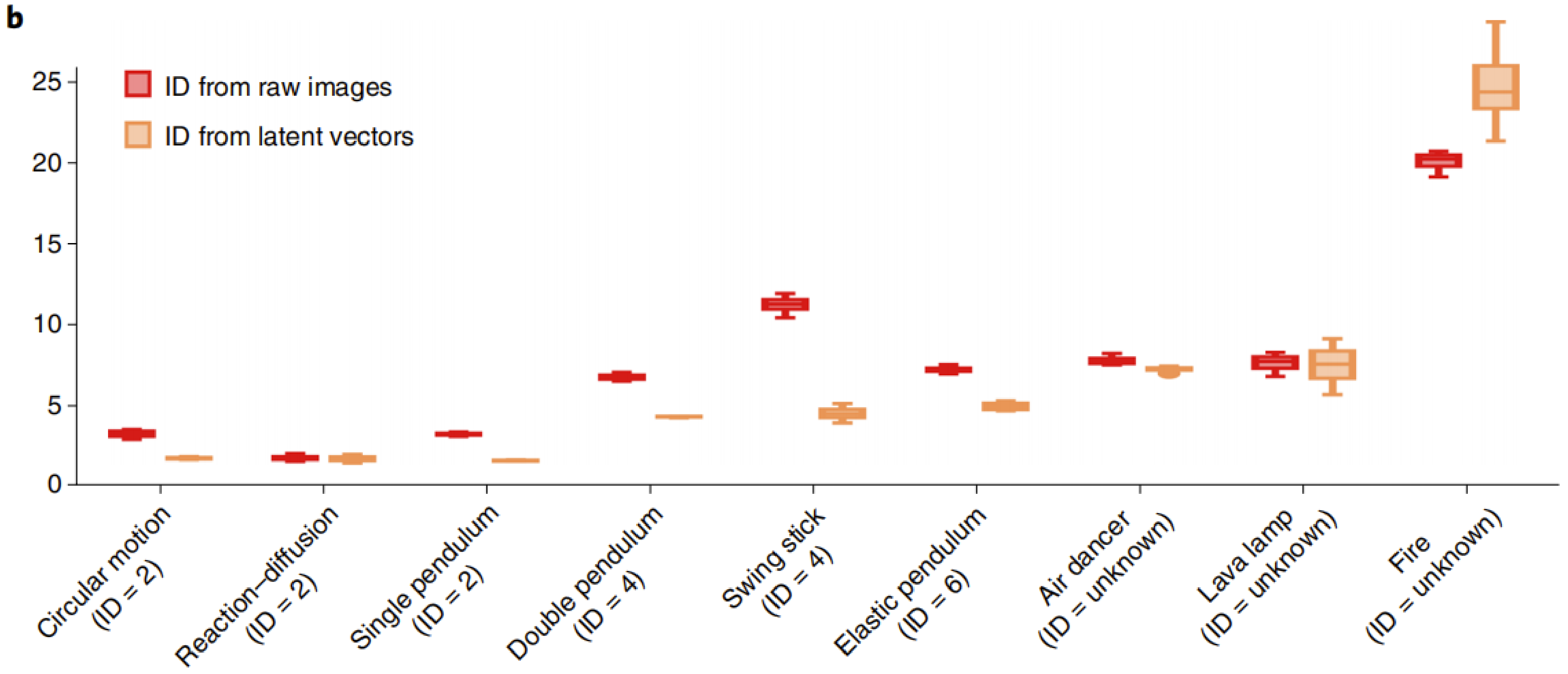


图 **2.** ID estimator results

2.4 Neural State Variables

We use a state variable $V \in \mathbb{R}^{\mathrm{ID}}$ to describe the dynamical system. We train a model to reconstuct the pretrained latent embedding from the aforementioned dynamics predictive model.

1. The input is $L_{t \to t+\mathrm{dt}}$.
2. The Encoder h_E operates as $V_{t \to t+\mathrm{dt}} = h_E(L_{t \to t+\mathrm{dt}})$
3. The Decoder $h_D \, \mathrm{operates\,as} \, \hat{L}_{t \to t+\mathrm{dt}} = h_D(V_{t \to t+\mathrm{dt}})$
4. The loss is

$$\mathcal{L} = \mathbb{E}_L[||h_D(h_E(L_{t \to t+\mathrm{dt}})) - L_{t \to t+\mathrm{dt}}||_2^2]$$

2.5 Hybrid prediction scheme

$$\hat{X}_{t+\mathrm{dt}} = g_D \circ h_D \circ h_E \circ g_E(\hat{X}_t)$$

3 Application

3.1 Neural State variables for stable long-term prediction

Two main challenge:

1. Non-iterative one-step prediction accuracy.
2. Long-term prediction stability.

Given a measure $M_S(\cdot)$ that measures the deviation of a predicted state from the true state space $\mathcal{S}$ and a prediction sequence $\{\widehat{X}_0, \ldots, \hat{X}_{\text{ndt}}\}$ from any initial space , we can quantify the stability of a prediction scheme as the growth rate of $M_S(\hat{X}_{\text{dt}})$ as a function of t.

We can use classical compute vision techniques to extract the conventional state variable, $M_{\mathcal{S}}^{\text{phys}}(\cdot)$ is defined as a binary value indicating whether the same set of physical variables can still be distilled from a predicted $\hat{X}$ as its corresponding ground-truth state. If so $M_{\mathcal{S}}^{\text{phys}}(\cdot)=1$, otherwise $M_{\mathcal{S}}^{\text{phys}}(\cdot)=0$.

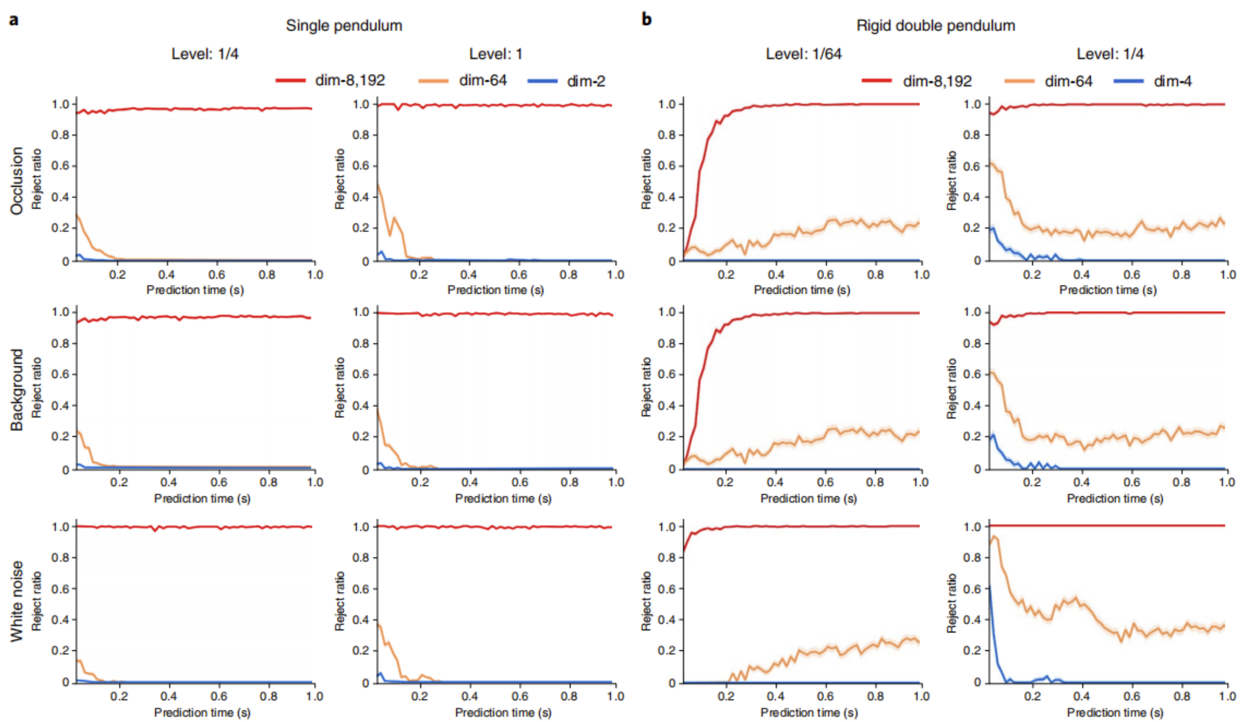


图 3. Neural state variables for robust long-term prediction.

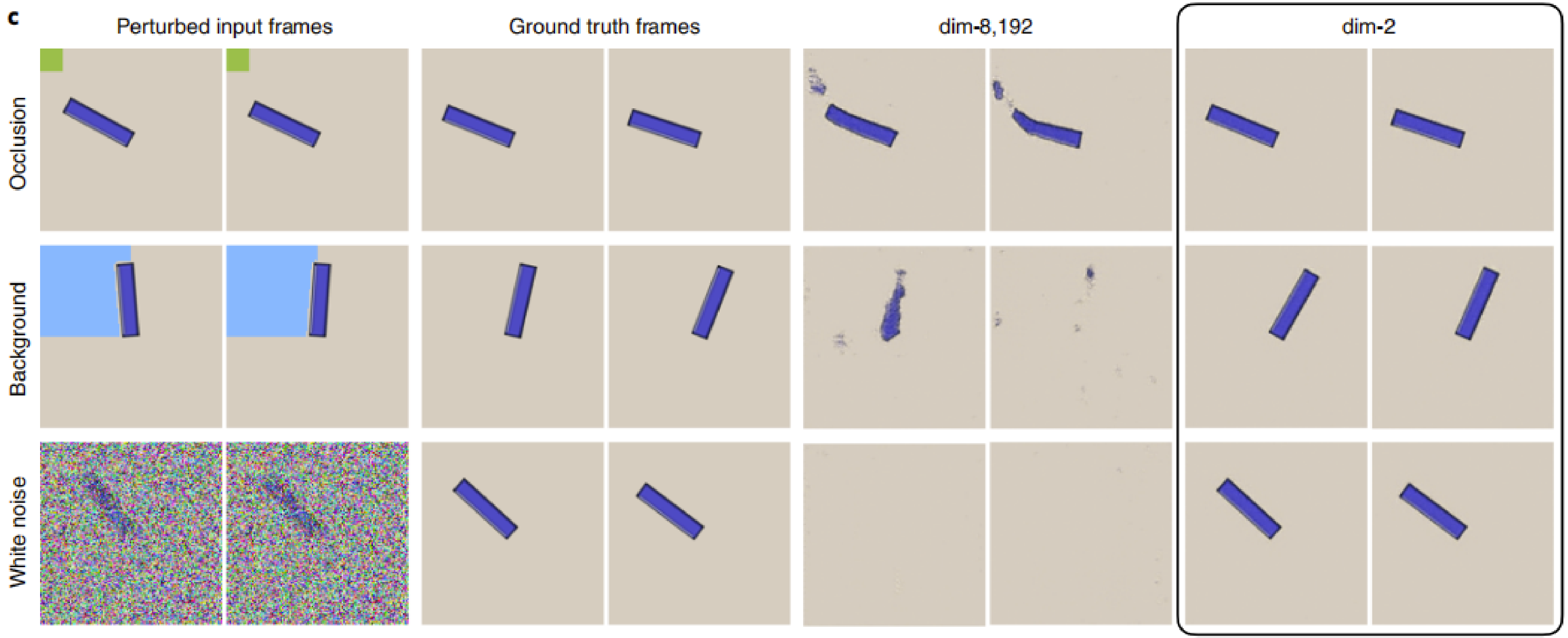


图 4. Neural state variables for robust long-term prediction.

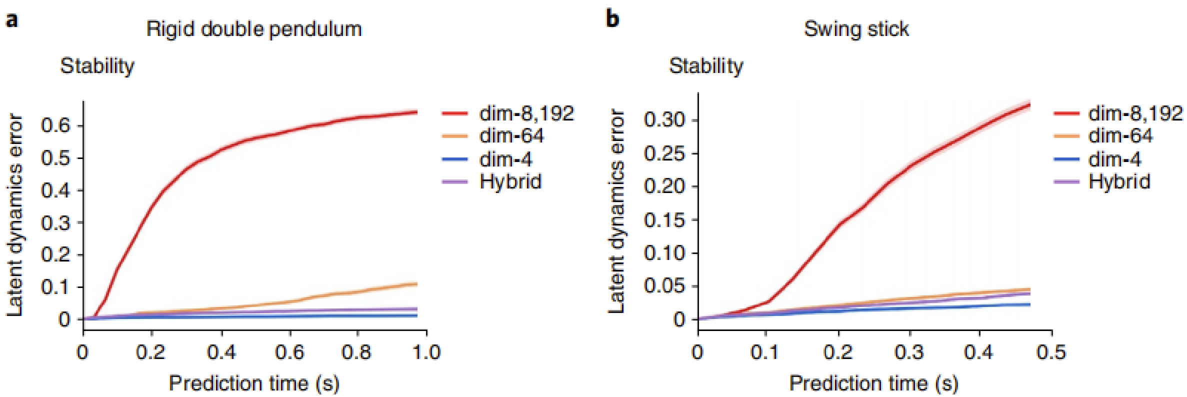
3.2 Neural state variables for dynamics stability indicators

However, in most of the video representations in our dataset we do not know either which variables to extract or how to extract them directly from videos.

$M_{\mathcal{S}}^{\text{neur}}(\cdot)$ is a metric on a pair of states $(\hat{X}_t, \hat{X}_{t+\text{dt}})$

$$M_{\mathcal{S}}^{\text{neur}}(\hat{X}_t, \hat{X}_{t+\text{dt}}) = |h_E \circ g_E(\hat{X}_{t+\text{dt}}) - \hat{F}_V(h_E \circ g_E(\hat{X}_t))|$$

where $\hat{F}_V$ is the NN approximate the latent dynamics $\hat{V}_{t+\text{dt}\to t+2\text{dt}} \leftarrow \hat{F}_V(V_{t\to t+\text{dt}})$, $h_E \circ g_E(\hat{X}_t) = \hat{V}_{t\to t+\text{dt}}, h_E \circ g_E(\hat{X}_{t+\text{dt}}) = \hat{V}_{t+\text{dt}\to t+2\text{dt}}$ are the neural state of $\mathbb{R}^{\text{ID}}$.



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Latent dynamics error versus reject ratio

System	Correlation
Single pendulum	97.33%
Rigid double pendulum	97.45%
Elastic double pendulum	98.76%

图 **5.** Neural state variables for dynamics stability indicators.