Characterizing information loss in a chaotic double pendulum with the Information Bottleneck

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Abstract

A hallmark of chaotic dynamics is the loss of information with time. Although information loss is often expressed through a connection to Lyapunov exponents valid in the limit of high information about the system state—this picture misses the rich spectrum of information decay across different levels of granularity. Here we show how machine learning presents new opportunities for the study of information loss in chaotic dynamics, with a double pendulum serving as a model system. We use the Information Bottleneck as a training objective for a neural network to extract information from the state of the system that is optimally predictive of the future state after a prescribed time horizon. We then decompose the optimally predictive information by distributing a bottleneck to each state variable, recovering the relative importance of the variables in determining future evolution. The framework we develop is broadly applicable to chaotic systems and pragmatic to apply, leveraging data and machine learning to monitor the limits of predictability and map out the loss of information.

1 Introduction

A fundamental aspect of chaos is the loss of information over time: for any measurement of a chaotic system with finite resolution, there is a finite time horizon beyond which the measurement bears no predictive power [22, 8, 26, 5, 11, 4]. The premise of this work is simple: to find the optimally predictive information in a chaotic system at different levels of granularity, and to study how the predictive power of this information erodes with the passage of time.

Information loss is intimately connected to the distortion of regions in phase space by chaotic dynamics, and thus to Lyapunov exponents: the sum of the positive Lyapunov exponents gives the Kolmogorov-Sinai (KS) entropy, the average rate of information loss[5]. However, these quantities are valid in the limit of maximal information—where infinitesimally-separated trajectories are discernible—and are thus somewhat removed from reality [5]. The (ϵ , τ)-entropy generalizes the KS entropy, describing the loss of predictive power for different amounts of information about the system state [9]. It is defined by way of a rate-distortion objective that minimizes the rate of information needed to predict the system state better than a threshold value of some chosen measure of distortion.

The Information Bottleneck (IB) is a rate-distortion problem where the measure of distortion is based on mutual information; it extracts the information from one variable that is most shared with a second variable [25]. We can use the IB to find optimally predictive information from one state of a chaotic system about a future state, and at the same time measure the loss of predictive power [6]. In this work we develop a framework that uses the IB for analyzing chaotic dynamics with machine learning. We

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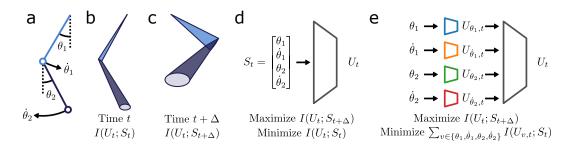


Figure 1: Predicting the future of a double pendulum given finite information. (a) The double pendulum system with four state variables $\theta_1, \dot{\theta}_1, \theta_2, \dot{\theta}_2$. (b) At time t the state S_t is measured, yielding a random variable U_t . The finite mutual information between the state and the measurement $I(S_t; U_t)$ manifests as a continuum of underlying states that cannot be discerned given an outcome of U_t . (c) Information is lost over time due to the double pendulum's chaotic dynamics. The representation U_t contains less information about the future state $S_{t+\Delta}$ than it does about the present state. (d) The measurement U_t is a function of S_t and can be learned with a neural network. To extract the information from the current state S_t most predictive of the future state, we optimize the Information Bottleneck objective. (e) By distributing bottlenecks, we gain marked interpretability by monitoring the share of optimally predictive information across state variables.

use an interpretable variant of the IB, the Distributed IB [15], to decompose the optimally predictive information in terms of a system's state variables.

2 Approach

Our testbed is a double pendulum (Fig. 1a): one of the simplest physical systems to exhibit chaotic behavior [23]. We simulated 10,000 trajectories at constant energy (details in the Appendix).

Given a random variable $S_t \sim p(s_t)$ for the system state at time t, a measurement U_t is any (possibly stochastic) function of the system state: $U_t \sim p(u_t|s_t)$. A measurement process shares mutual information $I(U_t; S_t)$ with the underlying state, defined as the reduction in Shannon's entropy [21] about S_t once U_t is known. For a continuous variable S_t and without infinite measurement capabilities, the outcome of U_t can only narrow down the possible values of S_t , which we visualize in Fig. 1b as a region of possible pendulum states. We can similarly examine the reduction in entropy about a future state after time Δ has elapsed, given the same measurement U_t . Then $I(U_t; S_{t+\Delta})$ serves as an upper bound of the predictive capabilities of any forecasting device given the outcome of the measurement U_t . The passage of time invariably expands our uncertainty about the system state (Fig. 1c).

Importantly, different measurements of the state—that is, different measurement processes U, not different outcomes u of the same measurement—can have identical $I(U_t; S_t)$ but vary in the information shared with the future state. We seek the measurement U_t that is most predictive of the future dynamics, for a given allowance of information about the present. To find this optimally predictive information, we use the Information Bottleneck [25, 3, 6] and optimize over the space of possible measurements. The following objective maximizes information about the future state and the information about the current state:

$$\mathcal{L}_{\mathbf{IB}} = \beta I(U_t; S_t) - I(U_t; S_{t+\Delta}). \tag{1}$$

The parameter β controls the bottleneck, restricting the information preserved about the present state.

As the bottleneck strength β varies, a trajectory in the "information plane" [24] is traced (Fig. 2a), which shows the exchange rate of information preserved about the present state versus information predictive of the future state, for different time horizons Δ . U_t can have no more information about $S_{t+\Delta}$ than it does about S_t , so no trajectory can exist above the line with slope 1. Optimal U_t are as close to this line as possible, and for a chaotic system longer time horizons are further displaced.

Measuring mutual information from data is notoriously tricky [20, 14, 17]. To be compatible with machine learning, the Variational Information Bottleneck (VIB) [2] replaces the mutual information terms of Eqn. 1 with bounds in a framework nearly identical to that of Variational Autoencoders [13, 10]. The bottleneck of Eqn. 1 is replaced with an upper bound on the mutual information,

$$I(U_t; S_t) \le D_{\mathbf{KL}}(p(u_t|s_t)||r(u)).$$

$$\tag{2}$$

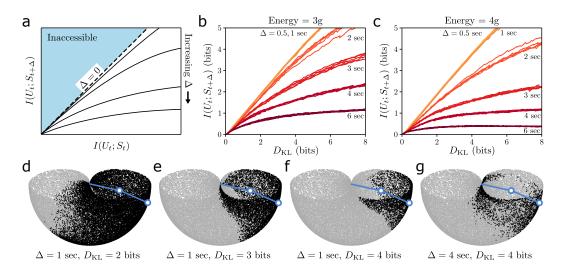


Figure 2: Optimally predictive information found by the Information Bottleneck. (a) The information plane compares the amount of information in U_t about the present and future states. Optimally predictive information then traces out trajectories that are determined by the decay of information in the dynamics. (b, c) We optimize the variational IB objective and display the trajectories for different time horizons, using the KL-divergence bound discussed in the text, for double pendulums with total energy 3g and 4g, respectively. The trajectories from five different splits of the training data are plotted for each Δ . (d-g) We visualize learned compressions of a particular pendulum state (overlaid; energy=3g) by displaying all other states (dots at the position of the second mass) that have a similar representation U_t . Gray dots show a random sample over all system states.

The Kullback-Leibler (KL) divergence— $D_{\text{KL}}(w(x)||z(x)) = \mathbb{E}_{x \sim w(x)}[-\log (z(x)/w(x))]$ quantifies the difference between the encoded distribution $p(u_t|s_t)$ and a prior distribution $r(u_t) = \mathcal{N}(0, 1)$ [13]. As the KL divergence tends to zero, all representations become indistinguishable from the prior and from each other, and therefore uninformative. We will use the KL divergence as a proxy for the amount of information contained in the measurement U_t .

To estimate the information with the future state, we employ the Noise Contrastive Estimation (InfoNCE) loss used in representation learning as a lower bound for the mutual information in Eqn. 1, $I(U_t; S_{t+\Delta}) \ge -\mathcal{L}_{InfoNCE}$ [16, 17] (the loss is reproduced in the Appendix). Instead of decoding the representation U_t to a distribution over $S_{t+\Delta}$, which would require discretization of a four-dimensional space, we learn an encoder for the future state and compare U_t to $V_{t+\Delta}$ in a shared representation space. The degree to which U_t can be matched with its future counterpart in the midst of distractor representations quantifies the amount of information they share.

3 Results and Discussion

As the time horizon increases, we find the expected trend in information plane trajectories (Fig. 2b,c): for a given amount of information about the present, less information is recoverable about the future. What are the optimal measurements U_t for different information allowances and time horizons? A measurement encodes a particular present state s into a distribution p(u|s) in embedding space; we visualize other states s' that have similar distributions and would therefore be difficult to distinguish given a particular measurement outcome u. We display in Fig. 2d-g scatter plots of the positions of the second pendulum mass for all states that are co-embedded at different information rates D_{KL} . Specifically, as all states are embedded to multidimensional Gaussian distributions, we use the Bhattacharyya coefficient [12]—0 for perfectly disjoint and 1 for perfectly matching distributions—to characterize the similarity between distributions, displaying all states with value greater than 0.5. The measurement process is therefore a clustering of states with similar fates after time Δ .

Visualizing the information content of the optimal measurements leaves much to be desired. We necessarily exclude several dimensions of the state, and can do little more than visual inspection. Instead, we seek a general method to interrogate the optimal information. We employ the Distributed

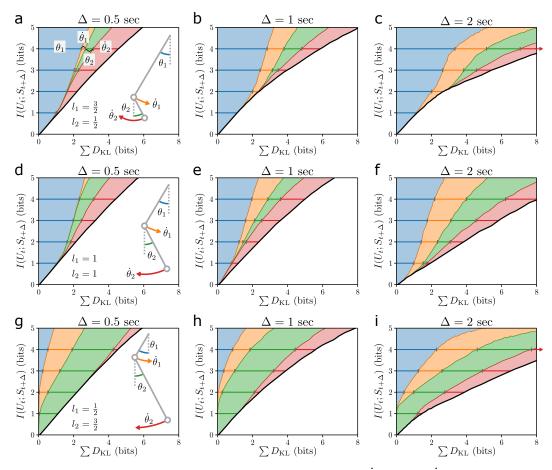


Figure 3: The distribution of predictive information over θ_1 , $\dot{\theta}_1$, θ_2 , and $\dot{\theta}_2$. In each plot, we display the information plane trajectory (black curve) found by optimizing the Distributed Information Bottleneck with a bottleneck on each of the state variables. At each point in the trajectory, we display the decomposition of the sum total KL-divergence, an upper bound on the information contained in U_t about the state S_t , in terms of the allocation to each of the four state variables. The pendulum arm length ratio varies across rows and the time horizon varies across columns.

Information Bottleneck [15, 7, 1], which modifies the optimization objective in 1 by distributing bottlenecks to each of the state variables (Fig. 1e). While maximizing the predictability of the future state as before, the variables are encoded independently and the sum of information is minimized. We acquire a degree of interpretability in the form of information allocation across the measurements, in exchange for less optimal measurements than can be found with the IB.

In Fig. 3, the information plane trajectories are decomposed in terms of the KL-divergence contribution from each of the state variables. Intuitively, a variable is encoded with a higher KL-divergence if it is more predictive of the future state, thereby granting insight into the relative role each variable plays in the dynamics. By changing the ratio of the arm lengths in the double pendulum, the variables pertaining to the longer arm become more informative about the future dynamics.

We have developed a framework to analyze the dynamics of a chaotic system through the lens of information theory using machine learning and data. The Information Bottleneck finds the optimally predictive information in a system state, and the Distributed IB confers interpretability about the role that each variable plays in the dynamics. The bounds on mutual information facilitate integration with off-the-shelf machine learning models and allow per-sample inspection of information allocation. The bounds are also the method's primary limitation: careful characterization of the mutual information bounds is necessary for any absolute measurements to be made (e.g., estimates of the Kolmogorov-Sinai or (ϵ, τ) entropy). Nevertheless, even with only relative measurements of information there is a rich source of insight into chaotic dynamics.

Impact statement

Machine learning struggles with interpretability [18, 19], complicating its application in the natural sciences and many other domains. In this work we have introduced a machine learning framework whose emphasis is on understanding a dynamical system. The Distributed Information Bottleneck offers a degree of interpretability in the form of information allocation across components of an input, thereby enhancing the utility of machine learning for the sciences.

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Checklist

1. For all authors...

- (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
- (b) Did you describe the limitations of your work? [Yes]
- (c) Did you discuss any potential negative societal impacts of your work? [No] We are not aware of any.
- (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
- 2. If you are including theoretical results...
 - (a) Did you state the full set of assumptions of all theoretical results? [N/A]
 - (b) Did you include complete proofs of all theoretical results? [N/A]
- 3. If you ran experiments...
 - (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes] Specifics for simulations and training are in Appendix A. We have included code with our submission and will post to Github upon acceptance.
 - (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] Appendix
 - (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] We included traces from five data splits in Fig. 2.
 - (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] Appendix
- 4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
 - (a) If your work uses existing assets, did you cite the creators? [N/A]
 - (b) Did you mention the license of the assets? [N/A]
 - (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
 - (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
 - (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
- 5. If you used crowdsourcing or conducted research with human subjects...
 - (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
 - (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
 - (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]

A Implementation

Code and further visualizations are available on the project website, distributed-informationbottleneck.github.io.

All experiments were run on a single computer with a 12 GB GeForce RTX 3060 GPU; a single annealing run with 50k steps (without evaluating on the validation set) took about six minutes.

Value
Leaky ReLU ($\alpha = 0.2$)
[128, 128]
[128, 128]
32
[256, 256]
64
[256, 256]
[1, 2, 4, 8, 16, 32, 64, 128]
256
Adam
3×10^{-4}
5×10^{-4}
2
5×10^4
Euclidean squared

Table 1: Training parameters for the IB and DIB experiments.

Simulations of the double pendulum were run using scipy.integrate.odeint, with a timestep $\Delta t = 0.001$ sec, masses of $m_1 = m_2 = 1$ kg, energy $E \in \{3g, 4g\}$, arm lengths $l_1, l_2 \in \{(1m, 1m), (1.5m, 0.5m), (0.5m, 1.5m)\}$, and a total simulation time of 100 sec. System states were saved every 0.02 sec.

For each pair of lengths of the pendulum arms l_1 , l_2 , we simulated 10,000 trajectories. Every starting state had zero kinetic energy and was created by randomly sampling the first pendulum arm's angle uniformly and then solving for the second arm's angle such that the system had the prescribed energy. The simulation was run for 100 sec, and was discarded if the energy ever deviated by more than 0.001 of the prescribed energy. Data for the first 50 sec was not used in order to minimize the effect of the initialization.

Training hyperparameters and architecture details are shown in Table 1. The only tuning that was done involved the annealing: we increased the number of training steps and decreased $\beta_{initial}$ until the trajectories were consistent. The optimization did not appear to be very sensitive to the other parameters (e.g., the architecture specifications).

A.1 InfoNCE loss

The InfoNCE comparison [16] is evaluated through the following loss contribution:

$$\mathcal{L}_{\text{InfoNCE}} = -\sum_{i}^{n} \log \frac{\exp(s(u_X^{(i)}, u_Y^{(i)})/\tau)}{\sum_{j}^{n} \exp(s(u_X^{(i)}, u_Y^{(j)})/\tau)},$$
(3)

where both sums run over a batch of n examples, s(u, v) is a measure of similarity (e.g., negative Euclidean distance), and τ acts as an effective temperature. Here X and Y refer generally to two random variables being matched; in this work they are S_t and $S_{t+\Delta}$, respectively.

Some intuition about the loss may be gained by viewing it as a classification task. Eqn. 3 is equivalent to a cross entropy loss when the correct classification for input $u_X^{(i)}$ is its counterpart $u_Y^{(i)}$, and prediction probabilities are a function of similarities in the shared representation space. (Specifically, the similarities are used as logits in the prediction, converted to probabilities with a softmax transform.) In other words, given a pair of instances and a batch of distractor instances, how well do the learned representations allow the pair to be correctly classified? If the best that can be done is excluding half the possible distractor instances, then there is about one bit of information between U_X and U_Y .