A RELATIONAL MACROSTATE THEORY GUIDES ARTIFICIAL INTELLIGENCE TO LEARN MACRO AND DESIGN MICRO

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October 19, 2022

ABSTRACT

The high-dimensionality, non-linearity and emergent properties of complex systems pose a challenge to identifying general laws in the same manner that has been so successful in simpler physical systems. In Anderson’s seminal work on why “more is different” he pointed to how emergent, macroscale patterns break symmetries of the underlying microscale laws. Yet, less recognized is that these large-scale, emergent patterns must also retain some symmetries of the microscale rules. Here we introduce a new, relational macrostate theory (RMT) that defines macrostates in terms of symmetries between two mutually predictive observations, and develop a machine learning architecture, MacroNet, that identifies macrostates. Using this framework, we show how macrostates can be identified across systems ranging in complexity from the simplicity of the simple harmonic oscillator to the much more complex spatial patterning characteristic of Turing instabilities. Furthermore, we show how our framework can be used for the inverse design of microstates consistent with a given macroscopic property – in Turing patterns this allows us to design underlying rule with a given specification of spatial patterning, and to identify which rule parameters most control these patterns. By demonstrating a general theory for how macroscopic properties emerge from conservation of symmetries in the mapping between observations, we provide a machine learning framework that allows a unified approach to identifying macrostates in systems from the simple to complex, and allows the design of new examples consistent with a given macroscopic property.

Keywords Emergence · macrostates · physics · complex systems · machine learning

1 Introduction

Among the most important concepts in physics is that of symmetry, and how symmetry-breaking at the microscale can give rise to macroscale behaviors. This deep connection was made clearest in the work of Noether \cite{1}, where she showed that for differentiable systems with conservative forces, every symmetry comes with a corresponding conservation law that describes macroscale behavior. An example is how time translation symmetry gives rise to the conservation of energy: simple harmonic oscillators conserve energy because, in the absence of friction, you will observe the same oscillation if starting a clock at the first cycle as at the thousandth – the behavior is time invariant. Thus, Noether’s theorem provided a means to relate laws – namely, regularities that are conserved (e.g., energy conservation) – to symmetries in the underlying physical system (e.g., time). Physics has been incredibly successful at discovering laws in this manner. However, so far, finding similar “law-like” behaviors for complex systems, such as biological and technological ones, has proved much more challenging because of their high-dimensionality, non-linear behavior, and emergent properties. Yet, the very concept of emergence provides a clue that such regularities should exist, even for complex systems. In Anderson’s seminal work on why “more is different” \cite{2}, he pointed to how symmetry-breaking also plays a prominent role in emergence: macroscale behaviors do not necessarily share all the same symmetries as the
Figure 1: Comparison between causal state theory, causal emergence theory and relational macrostate theories (A) In causal state theory, two microstates are equivalent (belong to the same macrostate) if their future microstate distributions are the same. (B) Causal emergence theory identifies macrostates where the past-future mappings are deterministic and non-degenerate at the macro scale, such that the macrostates can be distinguished from one another in the past (non-degeneracy) and the future (determinacy). Both causal state theory and causal emergence theory define macrostates in terms of temporal relations within a system of interest, as denoted by the square shape underlying the mapping. (C) In the relational macrostate theory we propose here, two microstates are equivalent if they relate to the same microstate distributions, which can be generalized to any type of relation, including past-future, rule-pattern, genotype-phenotype, etc. – the square and disk shapes denote that this is sufficiently general to apply to maps that exist across different spaces.

microscale laws or rules that give rise to them. While some of the symmetries are clearly lost, this also leaves open the possibility large-scale patterns that emerge will still retain other symmetries of the microscale rules. In addition to the rule-behavior mapping, there are other mappings unique to complex systems such as genotype-phenotype maps, text-image maps, etc., where symmetries may lead to conserved properties. The challenge to identifying general laws for complex systems then reduces to identifying which symmetries are preserved during the mapping – in general this is challenging because of their high dimensionality, suggesting that machine learning might be an approach that can aid in identifying conservation laws in these systems, if we can identify macrostates and the symmetries they retain from the microscale.

There have been several efforts focused on identifying macrostates associated with the emergent regularities found in complex systems [3, 4, 5]. Notably, Shalizi and Moore proposed causal state theory [6], which defines macrostates based on the relations between microstates. Here, two microstates are equivalent (belong to the same macrostate) if the future microstate distributions are the same (Figure 1A). Thus, the conserved symmetry is one pertaining to the prediction of future states. This, however, can exclude some well-defined macrostates in physics. For example, given a simple harmonic oscillator, two distinct microstates $u_1 = (p_1, x_1)$ and $u_2 = (p_2, x_2)$, where $p_1$ and $p_2$ are two observations of momentum and $x_1$ and $x_2$ there corresponding position, can have the same energy macrostate. However, their future microstate distributions will be different if $u_1$ and $u_2$ are not close to each other, say if, $u_1 = -u_2$. The conserved symmetry of Shalizi and Moore is therefore violated because this system does not retain predictability of future microstate distributions at the macroscale (because the macrostate of energy is related to the time translation symmetry, not the symmetry associated to predictability of future states).

If a proposed theory to define macrostates is not sufficiently general to include simple physical examples like the harmonic oscillator, it is unlikely to apply universally to complex systems. Indeed, Shalizi and Moore were not looking for a general theory of macrostates, but instead focused on the specific property of predictability of complex systems. Another approach was more recently proposed in causal emergence theory [7, 8, 9], which likewise has a specific goal in mind – to describe causal relations at the macroscale. Here, instead of using the properties of microstates, macrostates are defined based on the relations between macrostates by maximizing effective information at the macroscale. Effective information is the mutual information between two variables, under intervention to set one of them to maximum entropy (e.g., a uniform distribution over macrostates). Causal emergence occurs when the past and future of different macrostates are distinguishable (Figure 1B). Thus, the symmetry of distinguishing past and future leads to a conservation of distinguishability of macrostates.

Both causal state theory and causal emergence theory define macrostates in terms of temporal relations between past and future. However, not all regularities we might want to associate to laws involve time. For instance, to get the macrostates
of mass, force, and acceleration, physicists of past generations needed to study the relations between two objects rather than between points in time (past and future). This suggests that to develop a general theory of macrostates, these must be defined based on general relations between two observations (Figure 1C) that retain some of the symmetries of the underlying sets of observations – those observations could be objects, or points in time, as physics has already treated. But they can also be any other observation we can make with a measuring device, including more “complex” examples like genotype-phenotype maps, or word co-occurrence in language, or rule-behavior mapping necessary to describe patterning in biological form. As we will show, the theory of macrostates we propose is sufficiently general to extend to the symmetry of the microscale level rules (or laws), which allow us to identify sets of microscale rules that yield a given emergent, macroscale behavior.

When studying the history of the laws of physics, it is important to identify why the most successful laws have worked so well. Newton’s laws of motion work because there is a macroscale property called mass, which quantifies the amount of matter in each object, that reduces the description of the motion of high dimensional objects to a single measurable scalar quantity (mass) and its translation in $x, y, z$ coordinates. For complex systems it is not so obvious what the necessary dimensionality reduction will be that allows identifying law-like behavior, and it may vary from system to system. Of note, Newton’s laws cannot be developed in a world where mass can only be defined and measured in a few countable objects and is undefined or unmeasurable in others. In the current work, we show how artificial neural networks, themselves a complex system, can break the barrier of complexity to identify macrostates based on symmetries in complex systems. Existing machine learning methods such as contrastive learning, contrastive predictive coding, and word2vec have applied similar ideas to find lower dimensional representations for microstates by relations. However, these contrastive methods either require large numbers of negative samples that increases the cost of training, or only learning embeddings instead of functional mappings. Moreover, these methods are only useful for downstream tasks, which use the embedding trained by contrastive learning. Although we describe things at the macroscale, the world still runs on microscale features. This means we not only need to map microstates to macrostates, but that we need to provide an inverse path that samples microstate from a given macrostate. By developing the macrostate theory on general relations, and introducing invertibility, we propose a machine learning architecture, MacroNet, that can learn macrostates and design microstates.

In fact, a key feature of learning is demonstrating use cases of the knowledge learned. Therefore, to demonstrate how MacroNet is indeed learning the macrostates across of examples of simple physical systems and complex systems, we also use it to design new examples. There has been a flurry of recent work by scientists attempting to engineer AI scientists, and in particular AI physicists, that can learn the laws of nature from data with minimal supervision. Examples include: AI Feynman, which learns symbolic expressions; AI Poincare that can learn conservation laws; and Sir Isaac, an inference algorithm that can learn dynamical laws. Yet, science as done by scientists goes further than solely extracting laws from data – humans also implement that understanding in the real world. For example, in the case of Newton’s laws of motion, our knowledge of them has allowed us to engineer a range of systems, such as the design of airbags, racecars, airplanes, helicopters and even optimization of athlete performance, etc. Thus, we view the next advancement beyond artificial intelligence that can learn the rules by which data behave is AI that can also use that knowledge to design new examples of systems that will behave by the rules identified. A critical aspect of designing new examples of systems is identifying macrostate variables that reduce high-dimensional data to a few variables that capture the salient features. The invertibility of MacroNet not only allows the design of microstates sampled from an identified macrostate, but also provides a low-cost way to replace negative samplings in contrastive learning.

In what follows, we first introduce our mathematical framework for defining macrostates in terms of relations defined by symmetries in the data. Then, we propose a machine learning framework to find macrostates under the definition. For experiments, we first demonstrate the workflow of the framework by implementing it for linear dynamical systems. They are simple enough to demonstrate key concepts, but also exhibit rich behaviors. Then, we introduce the simple harmonic oscillator as a special case where macrostates are defined based on temporal relations, which demonstrates how our framework can extract familiar invariant macrostates (conserved properties associated to symmetries) from physics, such as energy. Finally, we turn to a real complex system, the macroscale Turing patterns that arise in diffusion reaction systems. We show how machine learning finds the macrostates associated with the emergent patterning in these systems, and then how this can be used to design microstates consistent with a target macroscale pattern.
2 Theory and Method

2.1 The relational macrostate theory that generalizable to the study of complex systems using neural networks

By definition, a macrostate is an ensemble corresponding to an equivalence class of microstates. Given a mapping \( \varphi_u \) that maps microstates to macrostates, two microstates \( u \) and \( u' \) belong to the same equivalence class if \( \varphi_u(u) = \varphi_u(u') \), that is if the microstates have the same behavior (macrostate) under the operation of the map. In this way, macrostates are also the parameters to describe distributions of microstates. This feature is a key reason why machine learning may be an optimal way to identify macrostates, particularly in cases of many-to-many mappings such as those that occur in rule-behavior maps, or under prediction with noise, both of which are characteristic of complex systems.

Here, we implement a formalism based on using relations arising due to symmetries to define macrostates. Consider two microstates \( u \in U \) and \( v \in V \) as two random variables. Their micro-to-macro relation can be mathematically represented as a joint distribution \( P(u, v) \). The \( u \) and \( v \) can be mapped to macrostates \( \alpha \) and \( \beta \) respectively by \( \varphi_u \) and \( \varphi_v \). So, we can also define micro-to-macro relation by the joint distribution \( P(\alpha, v) \) and \( P(u, \beta) \). For a given microstate \( u_i \) (or \( v_i \)), its micro-to-macro relation can be represented as a conditional distribution \( \Pr(\beta|u_i) \) (or \( \Pr(\alpha|v_i) \)).

Then, we can define macrostates in the most (relational) general case as:

**Definition 1.** Two pairs of microstates \( u_i \) and \( u_j \) (and \( v_i \) and \( v_j \)) belong to the same macrostate if and only if they have the same micro-to-macro relation:

\[
\begin{align*}
    u_i &\sim u_j \iff \Pr(\beta|u_i) = \Pr(\beta|u_j) \quad \text{(1)} \\
    v_i &\sim v_j \iff \Pr(\alpha|v_i) = \Pr(\alpha|v_j) \quad \text{(2)}
\end{align*}
\]

Note, this defines an equivalence class of symmetries where \( u_i \sim u_j \) and \( v_i \sim v_j \) (where \( \sim \) indicates “is equivalent to” under the symmetry operation). Thus, as in Noether’s theorem (and in Anderson’s formalization of emergence) we see that the definition of a macrostate entails simultaneously defining a class of symmetry operations, although here our definition is sufficiently general that the system of interest need not necessarily be continuously differentiable (as in the case of Noether’s theorem).
The definition can be approached by solving $\varphi_u(u) = \varphi_v(v)$ (see SI). This equation will be part of the loss function in the specified machine learning task of MacroNet. Since the macrostate of $U$ is defined by the macrostate of $V$, and vice versa, the solutions are not computed in a straightforward way, but must be calculated in relation to one another. As such, there can exist some inconsistent solutions. Figure 2A shows a consistent solution, however, Figure 2B shows an inconsistent solution. The points in red circles are classified into two macrostates, while they both have the same micro-to-macro relation. Not all consistent solutions are useful. If all microstates are mapped to the same macrostate, it still follows the definition, but this is a trivial solution and not informative, see Figure 2C. In addition to definition 1, we therefore require an information criterion to specify “good macrostates”. We do so by specifying a given dimension of macrostates, and then maximizing the mutual information $I(\varphi(v);\varphi(u))$ at the macroscopic level, where $(u,v)$ is sampled from $P(u,v)$. As a comparison, the effective information (EI) in causal emergence theory also uses the mutual information concept, but it has notable differences in how it is implemented beyond the fact that the theory presented here was designed for a machine learning implementation and causal emergence was not. In a discrete macrostate space, to quantify the causal effect, the EI re-assigns the marginal distribution of the macrostates with a uniform distribution. We do not make this requirement since we are not focusing on causal relations. Moreover, in a continuous macrostate space, the causal relation between macrostates may not make much sense because of the large number of different macrostates.

2.2 A self-supervised generative model for finding macrostates from observations

In the above formalization, a macrostate in $U$ is defined by macrostates in $V$ (i.e., macrostates are defined only in terms of their relations to other macrostates). This relational definition necessitates that we optimize the macrostate mapping iteratively to find an optimal solution. Thus, to implement the relational macrostates theory, we propose a self-supervised generative model for finding macrostates from observations (Figure 3A).

Our definition of macrostates can be achieved by optimizing macrostates to predict other macrostates. Here we use $\varphi_u$ and $\varphi_v$ to represent the coarse graining performed by the neural networks on $U$ and $V$ respectively. We have the prediction loss:

$$L_P = \mathbb{E}_{(u,v) \sim P(u,v)} |\varphi_u(u) - \varphi_v(v)|^2,$$

where $(u,v)$ are pairs of microstates sampled from the training data. The ideal solution for $\varphi$ is $\varphi_u(u) \approx_{\sigma} \varphi_v(v)$, meaning the macrostate of $u$ can be predicted by the macrostate of $v$ with error of $\sigma$, and vice versa. However, we need an additional term to avoid trivial solutions such as a low dimensional manifold or constant. To do this, we add a distribution loss, $L_D = L_{D_u} + L_{D_v}$, where:

$$L_{D_u} = \log P_{\text{normal}}(\varphi_u(u)) - \log \left| \det \frac{\partial \varphi_u(u)}{\partial u} \right|,$$

$$L_{D_v} = \log P_{\text{normal}}(\varphi_v(v)) - \log \left| \det \frac{\partial \varphi_v(v)}{\partial v} \right|.$$

The distribution loss is be minimized when the outputs follow independent normal distributions. We train the neural networks by combining the two loss functions:

$$L = L_P + \gamma L_D,$$

where $\gamma$ is the hyperparameter balancing the two loss terms. Combining these two terms, we can approach the mutual information criterion. Directly computing $L_D$ can be very expensive since it requires computing the Jacobian. However, since we want to do sampling, invertible neural networks (INNs) can help. The INNs are not only designed to be invertible, but also designed to easily compute the log-determinate of the Jacobian. The INNs will have the same output dimension as the input, so we abandon part of the dimensions (see SI S.3.c). For example, if we want to map an 8-dimensional vector to two-dimensional macrostate, the INNs will still give an 8-dimensional vector as a result, but we only take the first two variables as the macrostate for training. The abandoned six variables, however, still have been trained to follow independent normal distributions so we can do conditional inverse sampling.

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1We developed an invertible neural network python package – INNLab, available on GitHub: [https://github.com/ELIFE-ASU/INNLab](https://github.com/ELIFE-ASU/INNLab)
3 Results

In what follows we consider three explicit examples of the application of MacroNet. The first is a linear dynamical system, which allows us to demonstrate the key features of our workflow with a system that allows easily demonstrating key concepts, via the identification of a rotational symmetry and design of microstates consistent with this behavior. The second example is a simple harmonic oscillator (SHO), where we demonstrate MacroNet can identify a familiar symmetry and its corresponding macrostate in physics – time translation invariance and energy – by showing that our...
Figure 4: Training neural networks to find macrostates of linear dynamical systems. (A) the related pairs are parameters and trajectories. (B) by choosing an example trajectory, we can sample microstates of parameters or trajectories with the same macrostate. (C) Given the example trajectory (red dots), we can compute its macrostate. Then, we can sample parameters that have the sample macrostate. Using the sampled parameters, we can plot the trajectories generated by the sampled parameter (blue lines). (D) Using the same macrostate, we can sample an ensemble of trajectories that have the same macrostate.

3.1 Linear dynamical systems

We start with an experiment analyzing a linear dynamical system because these have many-to-many mappings. This allows us to demonstrate the workflow of identifying macrostates based on symmetries and then designing microstates from the identified macrostates. Here we choose a two-dimensional linear dynamical system whose dynamics are given by

\[ \frac{d\vec{x}}{dt} = M\vec{x}, \]

where \( \vec{x} \) is the independent variable, and \( M \) is a \( 2 \times 2 \) matrix that includes the parameters that specify the dynamics of the system. Given a matrix \( M \) and an initial state \( x_0 \), we can generate a sequence of observed states by computing \( x_{t+1} = x_t + Mx_t\delta t \). The trajectory will be \( T = [x_1, x_2, \ldots, x_n] \) in the two-dimensional space, where \( n = 8 \) and \( \delta t = 1/n \). Here we choose \( n = 8 \) because it is large enough to show the pattern of trajectories and not too large to slow the training. In this example, the micro-to-micro relations are represented by parameter-trajectory pairs, i.e., \((u, v) = (M, T)\). Note, in contrast to more standard approaches to studying dynamical systems, we are here not trying to find a macrostate by coarse graining the trajectory of states (which would depend on some variety of time symmetry, see introduction). Instead, we are coarse-graining to a macrostate that provides a map from parameters to observed
trajectories that will enable us to automatically generate new parameter-trajectory pairs that were not generated by running Eq 7.

We note the many-to-many mapping here means: 1) given one parameter, different initial states will lead to different trajectories. 2) sampling different parameters may lead to the same or similar trajectories. We use two neural networks to learn the macroscale relation between parameters and trajectories: one uses $\varphi_u$ to map the 4-d parameter matrix to a 2-d macrostate, and the other uses $\varphi_v$ to map the 16-d trajectory to a 2-d macrostate (Figure 4B), where we optimize to reduce the mutual information between the identified macrostates in both cases (Figure 4A).

After training, we can use the learned macrostates to design microstates. In Figure 4B, Given an example trajectory $T_e$, we can compute its macrostate $\beta = \varphi_v(T_e)$. The neural network $\varphi_u^{-1}$ samples parameters that can generate trajectories for the example microstate (Figure 4C). The sampled parameters follow a conditional distribution $P(M|\beta)$, where $M$ is the parameter matrix. In Figure 4D, we show how, given an anti-clockwise rotating trajectory, the parameters sampled all lead to anti-clockwise trajectories. By this process, we can design parameters of a system to mimic the behavior of any example, even without needing to translate the language describing the behavior to be human-interpretable. This ability has broad applicability for the design and control of complex systems, where simple mathematical descriptions have defied human scientists. Even when we do not know or have access to how we could describe a behavior, the neural network can still sample parameters to allow design of new examples through self-supervised learning.

So far, we have demonstrated sampling parameters for the matrix $M$, based on a specified macrostate (rotating anti-clockwise). We showed how the sampled parameters allow constructing new example trajectories using the sampled matrix $M$ in Eq 7 with the desired macroscale behavior. We can also sample trajectories directly, via a sampling process where we target the macrostate and then use the inverse sampling to recover trajectories. These sampled trajectories follow the distribution of $P(T|\beta)$, where $T$ is the trajectory microstate. Figure 4D show that the sampled trajectories all follow the same behavior, exhibiting anti-clockwise rotation, just as with the example trajectory. It is worth noting that here we never had to implement Eq 7 to generate the designed trajectories, but they were sampled directly from identification of the macrostate. We also did not give the neural network any concept of “rotate” or “clockwise”; the neural network discovered this symmetry on its own, as one that is relevant to how the parameters of the matrix $M$ map to observed trajectories. This experiment gives a simple example of how a neural network architecture like MacroNet can aid in identifying genotype-phenotype maps, where we genotypes play the role of parameters and phenotypes the role of trajectories.

3.2 Simple harmonic oscillators

Although we define macrostates on identifying symmetries underlying general relations, time relations are still of particular interest because of their long history in physics and their relationship to energy. Here, we demonstrate how MacroNet can automatically identify the symmetry of time translation invariance associated to energy, using a simple harmonic oscillator (SHO) as a case study. The Hamiltonian of SHOs is:

$$
\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2}kx^2.
$$

(8)

In this experiment, we let $m = 1$ and $k = 1$ for all cases. The micro-to-micro relation is a temporal relation, represented by pairs of $(x_0, p_0)$ and $(x_{\tau}, p_{\tau})$, where $x_0$ and $p_0$ are the initial position and momentum and $\tau$ is uniformly sampled time interval $(0, 2\pi)$ (see Figure 5A). Since we are trying to find a time invariant quantity, the mapping function $\varphi_u$ and $\varphi_v$ should not be different. So, we force the two neural networks $\varphi_u$ and $\varphi_v$ to share the same weights.

Figure 5 shows our training results. When we require the neural network to learn a one-dimensional invariant as a macrostate, the macrostate is exactly a function of energy (Figure 5B). Figure 5C shows samplings from macrostates to microstates. The same color represents microstates sampled from the same macrostate. The sampling shows how the neural network has identified three concentric circles, which correspond to the equal energy surfaces of the SHOs (Figure 5C), where the equation $p^2 + x^2 = H$ represents a circle with a radius of $\sqrt{H}$. Note that the uncertainty of $\tau$ makes it impossible to accurately predict the future microstates. In fact, the optimal prediction at any microstate will be zero if we optimize the MSE loss. However, using MacroNet, we can still predict the future macrostates and sample microstates from them. This is an example of how predictions at the microscale can fail, and how macrostates can help solving many-to-many mapping problems, such that predictions are still possible.

3.3 Turing patterns

Finally, we applied the same method on a complex system: Turing patterns. Here, we are using the Gray-Scott Model [19], a 2-d space that has two kinds of components, $a$ and $b$, which might, for example, correspond to two
We trained the neural network to map parameters and patterns to each other at macroscale (such that these will share the same macrostate). Figure 6A, we can sample parameters \( u \) and \( v \) so we can sample any parameters along these equivalence curves and generate Turing patterns with the user-specified macrostate. Here, \( D \) will have stronger effect on differences in macroscale behavior than \( F \). And additional feature is that observing the sampled parameters can also tell us the importance of different parameters. Their dynamics can be described by the differential equation:

\[
\frac{\partial u}{\partial t} = D_u \nabla^2 u - ab^2 + F(1 - a)
\]

\[
\frac{\partial b}{\partial t} = D_b \nabla^2 b + ab^2 - (F + k)b
\]

where \( D_u, D_b, F \) and \( k \) are four positive constants - these four parameters determine the behavior of the system. This model can generate a set of complex patterns, see Figure 6A. By finding macrostates mapping patterns to parameters, we can then in turn design related systems by specifying parameters that will yield user-specified patterns. Figure 6B shows, the sampled rules (set of four parameters) will generate similar patterns as the example patterns. This experiment shows that our method can design complex systems by sampling parameters that will generate patterns exhibiting the same equivalence class (sharing the same symmetry) will therefore lead to patterns that have the same macrostates, so we can sample any parameters along these equivalence curves and generate Turing patterns with the user-specified behavior.

And additional feature is that observing the sampled parameters can also tell us the importance of different parameters for specifying a target macroscale behavior. For example, as shown in Figure 6B, different macrostates have similar sampling on \( D_u \). However, on \( (F, k) \), different macrostates sample different parameters. This indicates that \( F, k \) will have stronger effect on differences in macroscale behavior than \( D_u \). This has implications for specifying control
parameters in designing complex systems. An example of interest is in pattern formation in regeneration \cite{20}, where a framework like MacroNet could identify the patterns controlling specific features of shape.

4 Discussion

Since Anderson published the seminal paper, \textit{More is Different}, it has been increasingly recognized that complex systems displaying emergent behaviors do not necessarily share the same symmetries as their micro-rules \cite{21}. That is, we know the mapping from a micro-rule to a large-scale system does not preserve all the symmetries of the micro-rule, due to symmetry breaking and perturbations from the environment. In some sense, this is the very definition of “emergence”. However, we might expect some symmetries to be retained such that micro-rules share at least a subset of their symmetries with any macroscale emergent behavior. Indeed, this is what we see in the experiments presented in this work. Each macrovariable can represent a type of symmetry: for instance, the energy of a simple harmonic oscillator represents how all states with the same energy are symmetric in time to others with that energy. In a more complex case, the macrostates of Turing patterns contain the information that is invariant under the mapping from parameter to pattern, even under external perturbations. The parameters that having the same macrostate are symmetric to each other because they all generate the patterns with the same macrostate. By finding the macrostates via the mutual information shared between ensembles of microstates, we can align the symmetries shared by the two sets of microvariables. This is a general framework for identifying macrostates as maps conserving the symmetries of systems: hence, while given “more is different” is true in most cases, we can still find examples of macrovariables that behave as “more is same” because they will retain underlying symmetries present at the microscale.

The process of finding macrostates can be considered as a prediction problem: that is, it is one of finding predictable variables of two related observations. There are no such variables if two observations have zero mutual information. Thus, if two observations have none-zero mutual information, we can use macrovariables (ensembles of microstates) to connect the two observations. In this way, one can consider macrostates as the instantiated mutual information mapping observations of one system to another (or a system to itself at a different point in time).

Across our experiments, we showed how macrostates can emerge from identifying predictive relations between two sets of observations. The parameter-trajectory relation leads to the macrostate of rotation and direction. The temporal relation between past and future leads to the macrostate energy in the simple harmonic oscillator. In the more complex case of Turing patterns, macrostates arise from parameter-pattern relationships. Thus, by adopting this relationalism idea, we can establish an approach targeting an ambitious question in the complex systems field: is it possible find general laws of complex systems? To address this question, one key task is to find a set of universal macrostates that can be found in most complex systems. And hence the laws of the universal macrostates can be considered as the general laws of complex systems. The method proposed in this work makes an initial step for this target – by finding macrostates from relations, the macrostates can be used on both sides of the relations (although they may be interpreted...
differently on either side of the relation). For instance, in the Turing pattern case, the macrostates are not only the macrostates of patterns, but also the macrostates of parameters. For future work, to find more universal macrostates, the framework may be extended from second-order relationship to higher-order relationships. Applying this method more generally to complex systems may reveal there are indeed universal general laws, or it may reveal that no map can apply to all systems – that is, that the laws of complex systems are unique to specific classes of system. In either case, the framework we have presented here, which offers an automated means for identifying general laws via symmetries in complex systems, offers new opportunities for asking and answering such questions.

Acknowledgement

We would like to acknowledge Dr. Cole Mathis, Dr. Daniel Czegel, Dr. Douglas G. Moore and Dr. Enrico Borriello from the Walker lab at Arizona State University for suggestions and discussions. We thank Prof. Yi-Zhuang You from UCSD for his valuable suggestions on machine learning, Prof. Yunbo Lu from Tongji University for his support on computational resources, and Prof. Leroy Cronin from University of Glasgow for research support. This project was supported by a grant from the John Templeton Foundation.

Author Contributions

Y.Z. and S.I.W. developed the theory and designed the formalism. Y.Z. implemented the MacroNet machine learning architecture and performed the analyses. Y.Z. and S.I.W. wrote the manuscript.

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