Equivalence Class Learning for GENERIC Systems

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Abstract

In recent years, applications of neural networks to the modeling of physical phenomena have attracted much attention. This study proposes a method for learning systems that are described by the GENERIC formalism, which is a combination of analytical mechanics and non-equilibrium thermodynamics. GENERIC systems admit the energy conservation law and the law of increasing entropy under certain conditions. However, designing neural network models that satisfy these conditions is difficult. In this study, we introduce a relaxation model of the GENERIC form, thereby introducing an equivalence class into the set of models. Because the equivalence class of the target model includes a model that can be learned by neural networks, the learned model has the energy conservation law and the law of increasing entropy in high accuracy with respect to the true energy and the true entropy.

1. Introduction

Deep learning methods for learning physical equations have been studied extensively in recent years. Hamiltonian neural networks (Greydanus et al., 2019) are well known as a representative example. This method aims to learn the equations of motion in Hamiltonian dynamics, called the Hamilton equation, from data. Although the method has been extended in various ways, to the best of the authors' knowledge, GFINNs (Zhang et al., 2022) based on the GENERIC (Öttinger, 2018) formulation is the only one that has been proposed for learning non-equilibrium thermodynamics.

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Workshop on New Frontiers in Learning, Control, and Dynamical Systems at the International Conference on Machine Learning (ICML), Honolulu, Hawaii, USA, 2023.

The GENERIC (general equation for the non-equilibrium reversible-irreversible coupling) formulation is one of the theoretical frameworks of non-equilibrium thermodynamics. Other known theories of non-equilibrium thermodynamics include Onsager's theory based on the minimum damping principle (Onsager, 1931) and Yoshimura's theory based on Dirac dynamics (Yoshimura & GayBalmaz, 2018). Among these, the GENERIC formulation provides a general mathematical framework for describing non-equilibrium states of thermodynamic systems, which can simultaneously describe the reversible and irreversible partial dynamics of the system. GENERIC formulation is described by

$$\frac{\mathrm{d}u}{\mathrm{d}t} = L\frac{\partial E}{\partial u} + M\frac{\partial S}{\partial u}, \tag{1}$$

where u is a state variable. The variables E and S are the total energy and entropy variables represented by the variable u, and L and M are the operators or matrices that depend on u. It is known that if the algebraic conditions

$$L\frac{\partial S}{\partial u} = 0, \quad M\frac{\partial E}{\partial u} = 0 \tag{2}$$

are satisfied, then we have the conservation law of energy $\mathrm{d}E/\mathrm{d}t = 0$ and the law of increasing entropy $\mathrm{d}S/\mathrm{d}t \geq 0$. For this condition, L and M must be degenerate, which is often given in the following form:

$$L = \left(\begin{array}{c|c} * & O \\ \hline O & O \end{array}\right), \; M = \left(\begin{array}{c|c} O & O \\ \hline O & * \end{array}\right). \tag{3}$$

To learn a model based on (1) using neural networks from observed data, we need to learn the energy E, the entropy S, and the matrices L and M. In particular, when the matrices L and M are learned from data, the condition (2) must be satisfied in order for the energy conservation law and the law of increasing entropy to hold; however, hard-coding these conditions into the architecture of the model is difficult.

In this study, we propose a method to solve this problem. The basic idea is to introduce a new system that relaxes the GENERIC formulation. This system contains the GENERIC form, but has a degree of freedom in formulation, and is designed so that multiple energy and entropy functions give the same dynamics. This degree of freedom allows us to define an equivalence class for the set of energy

and entropy functions. The proposed method searches for a model within this equivalence class. As a result, although the learned model does not directly satisfy the condition (2), it can be proved that there exists an equivalent to the learned model that is a GENERIC system and satisfies (2). Since this hidden model is a GENERIC model that reproduces the data, the laws of energy and entropy hold. Therefore, if the hidden model is learned with sufficient accuracy, the dynamics of the hidden model, and thus the dynamics of the proposed model, will have the energy conservation law and the law of the increasing entropy of the true model.

Main contributions of this paper include:

- The first equivalence class learning method for deep physical models with physical laws.
- Learning of unknown GENERIC structures by Kernel-aware positive semi-definite matrix learning.

2. Related Work

Analytical mechanics is classified into Lagrangian mechanics and Hamiltonian mechanics (Abraham & Marsden, 2008; Arnol'd, 2013; Marsden & Ratiu, 2013), and in recent years, several neural network models for the equations of motion were proposed (Cranmer et al., 2020; Lutter et al., 2019). For learning a differential-equation model for dynamical systems from data, the neural ordinary differential equation (NODE, Chen et al. (2018)) is a typical method. NODE models the time-derivative of the states, thereby defining an ordinary differential equation (ODE) in a general way. However, this model cannot admit the energy conservation law because of the universality of neural networks. For physical modeling, models that preserve the laws of physics are preferred. The reversible contribution in the GENERIC formulation is generally assumed to be of the Hamiltonian form. For the Hamiltonian systems, some models are known (Chen et al., 2021; Matsubara et al., 2020; Zhong et al., 2019; Chen et al., 2019; Jin et al., 2020), for learning the energy function H using neural networks. GFINNs is a known method for learning GENERIC systems. In this method, the conditions (2) are added as regularization terms to the loss function. However, the regularization terms do not always vanish completely and these physical laws may not be satisfied.

3. Proposed Model: Relaxation of GENERIC Forms and Equivalence Classes of Systems

Equations in GENERIC form are usually rewritten in the form (3) when transformed to the appropriate coordinate system. First, let us briefly explain why the form is derived in this way. The condition (2) means $\nabla E \in \mathrm{Ker}\ M$ and $\nabla S \in \mathrm{Ker}\ L$. In particular, focusing on $\nabla E \in \mathrm{Ker}\ M$, we decompose the phase space as $\nabla M \oplus (\mathrm{Ker}\ M)^\perp$. where $(\mathrm{Ker}\ M)^\perp$ is the orthogonal complement of $\mathrm{Ker}\ M$. Since $\nabla E \in \mathrm{Ker}\ M$, the domain of L is effectively $\mathrm{Ker}\ M$. Similarly, the domain of M is effectively $(\mathrm{Ker}\ M)^\perp$. M is a symmetric matrix and can be diagonalized by an orthogonal matrix. Each column of the orthogonal matrix is an eigenvector of M. In particular, those corresponding to eigenvalue 0 are the basis of $\mathrm{Ker}\ M$, and other eigenvectors are the basis of $(\mathrm{Ker}\ M)^\perp$. Therefore, when these eigenvectors are rearranged into bases, the GENERIC system takes the form (3). In other words, in general, the GENERIC system (1) can be written in the following form:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = L\Pi_{\mathrm{Ker}M}\nabla E + M\Pi_{(\mathrm{Ker}M)^\perp}\nabla S, \tag{4}$$

where, $\Pi_{\mathrm{Ker}M}$ and $\Pi_{(\mathrm{Ker}M)^\perp}$ are the projection operators onto $\mathrm{Ker}\ M$ and $(\mathrm{Ker}\ M)^\perp$, respectively.

We now relax the condition (2). Specifically, we consider systems that can be written in the form (4) but do not satisfy (2). We define the following equivalence relation on the set of such a system, or more precisely, on the set of E and S when L and M are fixed.

Definition 3.1. Fix L and M in (4). For a set $\mathcal{S} = \{(E, S)\}$ of pairs of functions E and S, if (E_1, S_1) and (E_2, S_2) determine the same u_t by (4), (E_1, S_1) and (E_2, S_2) are defined to be equivalent. The equivalence class defined by (E, S) is denoted by $[(E, S)]$.

Theorem 3.2. *For a GENERIC system $(E_\mathrm{G}, S_\mathrm{G})$, any system in its equivalence class $[(E_\mathrm{G}, S_\mathrm{G})]$ has the conservation law of E_G and the increasing law of S_G.*

Proof. Let u be a state variable of the system (4) with $(E, G) \in [(E_\mathrm{G}, S_\mathrm{G})]$, and u_G be that of (4) with $(E_\mathrm{G}, S_\mathrm{G})$. Since, these two systems are equivalent, $\mathrm{d}u/\mathrm{d}t = \mathrm{d}u_\mathrm{G}/\mathrm{d}t$. Hence, $\frac{\mathrm{d}E_\mathrm{G}(u(t))}{\mathrm{d}t} = \nabla E_\mathrm{G} \cdot \frac{\mathrm{d}u}{\mathrm{d}t} = \nabla E_\mathrm{G} \cdot \frac{\mathrm{d}u_\mathrm{G}}{\mathrm{d}t} = 0$. The law of increasing entropy can be shown in the same way. □

This theorem implies that there exist multiple E, G that give the same dynamics as the the dynamics of E_G, S_G, which is the degree of freedom explained in Section 1. Hence, if we can learn a system (E, S) in the equivalence class $[E_\mathrm{G}, S_\mathrm{G}]$ of the target GENERIC system $(E_\mathrm{G}, S_\mathrm{G})$, then this system may not have the conservation and increasing laws for (E, S), but it does for the true system $(E_\mathrm{G}, S_\mathrm{G})$ and hence should have good long-term prediction performance.

Now, consider a learning model based on (4). Assume that L, M, E, and S are all unknown. E and M are modeled by neural networks E_NN and S_NN. To construct the projection operator that appears in (4), we need $\mathrm{Ker}\ M$. Therefore, the proposed equivalence learning technique can be applied to the existing models by computing the kernel of the matrices

L and M; however, here we consider a method to learn the matrix M, being aware of the basis of $\mathrm{Ker}\ M$.

To this end, we use the fact that M can be decomposed into $M = P\,\mathrm{diag}(\lambda_1, \dots, \lambda_k, 0, \dots, 0)\,P^\top$, where P is an orthogonal matrix, k is the rank of M, and $\lambda_1, \dots, \lambda_k$ are non-negative eigenvalues of M, as explained in the above. These P and λ_j's are functions of the state variable u, and hence we try to learn them using neural networks.

First, basically, λ_j's can be learned with typical multilayer perceptrons; the output is guaranteed to be non-negative by applying the ReLU function. In addition, to guarantee $\mathrm{Ker}\ M \neq \emptyset$, some of eigenvalues must be zero. For simplicity, we assume that the first k eigenvalues are non-zero. If the value of k is not known, we can try various values of k and employ the one with the best performance. In this paper, we let λ_j's be sparse and determine the value of k by the neural network λ_{NN}.

Next, for learning the orthogonal matrix P, a simple method is to add $\|P^\top P - I\|$ to the loss function; however, $\|P^\top P - I\|$ is not always completely zero, and P may not be orthogonal. Therefore, we use the fact that the set of orthogonal matrices has the structure of a Lie group. Because the corresponding Lie algebra is the set of skew-symmetric matrices P is learned as the exponential of a skew-symmetric matrix. Specifically, A_{NN} is a $n \times n$ matrix represented by a neural network, and P is learned by $P_{\mathrm{NN}} = \exp(A_{\mathrm{NN}} - A_{\mathrm{NN}}^\top)$. Learning in this way, the columns of P_{NN} corresponding to the eigenvalue 0 become the basis of $\mathrm{Ker}\ M$, and the other columns become the basis of $(\mathrm{Ker}\ M)^\perp$. The projection matrix can be constructed by using these: $\Pi_{\mathrm{Ker}M_{\mathrm{NN}}} = P\,\mathrm{diag}(\underbrace{0, \dots, 0}_{k}, \underbrace{1, \dots, 1}_{n-k})\,P^\top$, $\Pi_{(\mathrm{Ker}M_{\mathrm{NN}})^\perp} = P\,\mathrm{diag}(\underbrace{1, \dots, 1}_{k}, \underbrace{0, \dots, 0}_{n-k})\,P^\top$.

Regarding the matrix L, because L must correspond to the Hamilton equation, the inverse of the restriction of L to the domain of L must be a symplectic form. Hence, we apply the method for learning symplectic forms proposed in (Chen et al., 2021).

Altogether, the proposed model is as follows:

$$
\begin{aligned}
&\frac{\mathrm{d}u}{\mathrm{d}t} = \tilde{L}\nabla E_{\mathrm{NN}} + \tilde{M}\nabla S_{\mathrm{NN}}, \quad \tilde{L} = \Pi_{\mathrm{Ker}\tilde{M}}^\top \hat{W}_u^{-1} \Pi_{\mathrm{Ker}\tilde{M}},\\
&\tilde{M} = P_{\mathrm{NN}}\mathrm{diag}(\lambda_{1,\mathrm{NN}}, \dots, \lambda_{k,\mathrm{NN}}, 0, \dots, 0)P_{\mathrm{NN}}^\top,\\
&P_{\mathrm{NN}} = \exp(A_{\mathrm{NN}} - A_{\mathrm{NN}}^\top),\\
&(\hat{W}_u)_{i,j} = \frac{\partial (Y_{\mathrm{NN}})_i}{\partial u_j} - \frac{\partial (Y_{\mathrm{NN}})_j}{\partial u_i}.
\end{aligned} \tag{5}
$$

In the model, the subscript NN indicates that the quantity is modeled by a neural network; tilde is the quantity created using the quantity modeled by the neural network.

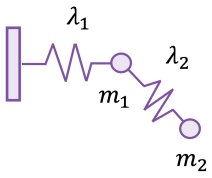


Figure 1. A thermoelastic double pendulum.

Assuming that time series data of state vectors $\{u^{(l)}\}$ and time-derivatives $\{\mathrm{d}u/\mathrm{d}t^{(l)}\}$ are given, the proposed model is trained by minimizing the squared error between the left-hand and right-hand sides of (5): $\|\frac{\mathrm{d}u}{\mathrm{d}t} - (\tilde{L}\nabla E_{\mathrm{NN}} + \tilde{M}\nabla S_{\mathrm{NN}})\|_2^2$.

4. Numerical Examples

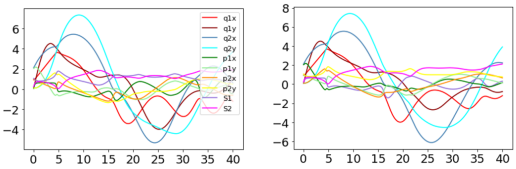
We performed some experiments to check if the proposed model certainly admits the energy conservation law and the law of increasing energy. Note that since the equivalence class learning can be applied to existing methods, no comparison with other models was made.

In the experiments, dense neural networks that had two hidden layers of 200 units were used for modeling the unknown quantities. In these layers, the hyperbolic tangent function is used as the activation function. In addition, the ReLU function is used to guarantee that the eigenvalues of M_{NN} are all non-negative. We used 80 percent of collected data for training and the remaining of the data for the test. We trained each model 10 times using Adam optimizer with a learning rate of 10^{-3} for 2000 iterations in the other two experiments. We performed our experiments on NVIDIA RTX A5000 with single precision. For the predictions after training, we used SciPy odeint under the default setting.

4.1. Thermoelastic Double Pendulum

We first consider a two-dimensional thermoelastic double pendulum shown in Figure 1. This system consists of two point masses m_1 and m_2 connected by thermoelastic springs of internal energy of E_1 and E_2. The positions and the momentums of the masses are denoted by q_1 and q_2 and p_1 and p_2, respectively. The entropy of two springs are denoted by S_1 and S_2. The state variables u is $u = (q_1, q_2, p_1, p_2, S_1, S_2)$, where $q_i, p_i \in \mathbb{R}^2$. The total energy E of the system is $E(u) = \| p_1 \|^2/2 + \| p_2 \|^2/2 + E_1(l_1, S_1) + E_2(l_2, S_2)$, where l_1 and l_2 are the lengths of the two springs: $l_1 = \|q_1\|, l_2 = \|q_2 - q_1\|$, the internal energy E_1 and E_2 of i-th spring is defined as $E_i = \frac{1}{2}(\log l_i)^2 + \log l_i + \mathrm{e}^{S_i} - \log l_i - 1$, and the total entropy S of the system is given by $S(u) = S_1 + S_2$. This model captures the simplest thermal effects: the internal energy should account for the stretches caused by

temperature changes. We generated 100 trajectories from $t_0 = 0$ to $t_T = 40$ with $\Delta t = 0.1$, whose initial conditions are sampled uniformly from $[0.9, 1, 1] \times [-0.1, 0.1] \times [2.1, 2.3] \times [-0.1, 0.1] \times [-0.1, 0.1] \times [1.9, 2.1] \times [0.9, 1, 1] \times [-0.1, 0.1] \times [0.9, 1, 1] \times [0.1, 0.3]$.

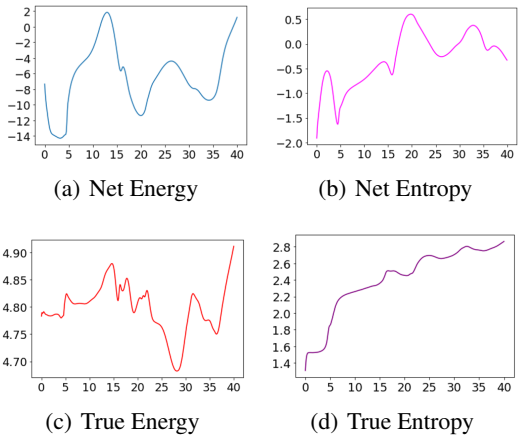


(a) Ground Truth (b) Prediction

Figure 2. Trajectories predicted by the proposed model for the double pendulum. The horizontal axis represents time.

The training and testing losses were 1.2484×10^{-5} and 1.4821×10^{-5}, respectively. The ground truth of the trajectory of the state variables and the predicted trajectory are shown in Figure 2. The prediction by the proposed model is very similar to the true trajectory.

Since the degeneracy conditions of GENERIC are relaxed, so neither the net energy E_{NN} nor the net entropy S_{NN} follows the laws of physics, as shown in Figure 3. However,



(a) Net Energy (b) Net Entropy

(c) True Energy (d) True Entropy

Figure 3. Time evolution of the net energy E_{NN}, the net entropy, the true energy and the true entropy obtained by the proposed model for the thermoelastic double pendulum system. The horizontal axis represents time.

the true energy changes in a small range. In addition, the entropy certainly keeps increasing. Therefore the true energy and true entropy both follow the laws of physics within a small error range. Note that a rigorous evaluation of the conservation of the energy and the increase of the entropy is difficult because these laws of physics hold within the modeling error, but the modeling error is computed as the mean squared loss of the time-derivative $\mathrm{d}u/\mathrm{d}t$, which is not of the energy or the entropy.

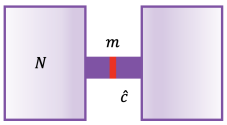
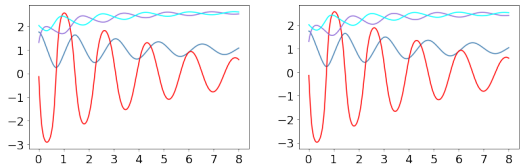


Figure 4. Two gas containers exchanging heat and volume.

4.2. Two Gas Containers Exchanging Heat and Volume

Secondly, we applied the proposed model to the two ideal gas containers, which are allowed to exchange heat and volume by a moving wall in the middle, as shown in Figure 4. This system has $u = (q, p, S_1, S_2)$, where q and p represent the position and momentum of the moving wall, while S_1 and S_2 are the entropies of the gases in the two containers. The total energy is $E = p^2/2m + E_1 + E_2$, where the energy of gas in the i-th container is $E_i = (\mathrm{e}^{\frac{S_i}{Nk_B}}/\hat{c}V_i)^{\frac{2}{3}}$, $V_1 = q$, $V_2 = 2 - q$, $\hat{c} = (4\pi m/3h^2N)^{\frac{3}{2}}\frac{\mathrm{e}^{\frac{5}{2}}}{N}$, where m represents the mass of the wall, N is the quantity of gas particles, h is the Planck constant and k_B is the Boltzmann constant. In our experiments, m, N, k_B and $\hat{c}$ are fixed to 1. The total entropy S is $S(u) = S_1 + S_2$. The training and testing losses



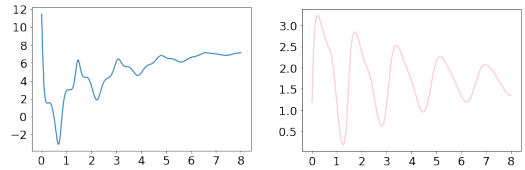
(a) Ground Truth (b) Prediction

Figure 5. Trajectories predicted by the proposed model for the two gas containers system. The horizontal axis represents time.

of this experiment were 4.8198×10^{-5} and 5.1721×10^{-5}, respectively. The predicted trajectory is shown in Figure 5. The behaviors of the energies and the entropies are shown in Figure 6. Regarding the real energy, although it seems that it is decreasing, the amplitude of the vibration is gradually decreasing and with a high probability in a long time prediction, it will converge. Therefore the model may satisfy the law of energy conservation after a long period. We will examine it in future work. The entropy keeps increasing also.

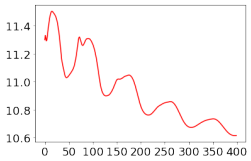
5. Concluding Remarks

In this paper, we have proposed the equivalence class learning for GENERIC systems. Since the condition (2) is relaxed this model does not satisfy the laws of physics for the energy and entropy modeled by the neural network, but does satisfy these laws for the true energy and entropy. This method can be combined with existing methods; however,

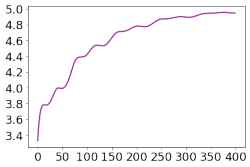


(a) Net Energy

(b) Net Entropy



(c) True Energy



(d) True Entropy

Figure 6. Time evolution of the net energy, the net entropy, the true energy and the true entropy obtained by the proposed model for the two gas containers system. The horizontal axis represents time.

combining this idea with various models and comparing their performance is future work. A rigorous evaluation method for the conservation of E and the increase of S is also a future issue.

Acknowledgements

Funding in direct support of this work: JST CREST Grant Number JPMJCR1914, JST PRESTO Grant Number JPMJPR21C7 and JSPS KAKENHI Grant Number 20K11693 and JSPS 23KJ1555.

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