SPARSE REPRESENTATION OF KOOPMAN OPERATOR

Yuya Note
Department of Electrical and Electronic Engineering
Kobe University
Kobe, Japan

Takaharu Yaguchi
Department of Mathematics
Kobe University
Kobe, Japan
yaguchi@pearl.kobe-u.ac.jp

Toshiaki Omori
Department of Electrical and Electronic Engineering
Kobe University
Kobe, Japan
omori@eedept.kobe-u.ac.jp

ABSTRACT

In this paper we propose a method for estimating dynamical systems using a sparse representation of the Koopman operator. The Koopman operator is inherently considered with infinite dimensional observables. The proposed method imposes a sparse constraint on the elements of the matrix that approximates the Koopman operator. Experiments on nonlinear dynamical systems showed that the proposed method was more accurate than the unconstrained method when the number of observables was large. It is also shown that the Koopman operator is sparsely estimated with more zero elements.

Keywords Sparse Modeling, Koopman Operator, Nonlinear Dynamical System

1 Introduction

In recent years, advances in measurement and computational techniques have improved the quality of data, and also the quantity of data has become enormous. These developments have led to a focus on data-driven approaches to extracting the structure and properties of systems from data. Data-driven approaches are important approaches for a variety of disciplines [1, 2], including natural sciences such as earth sciences [3, 4, 5, 6, 7] and neuroscience [8, 9], and for engineering disciplines such as fluid engineering [10, 11, 12, 13] and thermal engineering [14, 15].

Nonlinear dynamical systems are often used to describe natural phenomena and engineering systems due to their ability to model complex or highly interrelated behavior that is difficult to represent in linear dynamics. Because nonlinear dynamical systems are represented by nonlinear functions, the correspondence between inputs and outputs becomes complex, making it difficult to predict and analyze their behavior.

In the analysis of nonlinear dynamical systems, the Koopman operator has attracted much attention [16, 17, 18, 19, 20, 21, 22, 23]. The Koopman operator is a linear operator introduced for nonlinear dynamics. The Koopman operator generally requires consideration of an infinite-dimensional function space, including a function called an observable, but for actual calculations the Koopman operator must be approximated in a finite dimension. Therefore, when using the Koopman operator, the choice of functions as observables is important.

In this paper we propose a method for estimating dynamical systems using a sparse representation of the Koopman operator. This method imposes a regularization on the magnitude of the corresponding coefficient for each observable and performs sparse estimation. The results demonstrated that this method can achieve accurate estimation in long-term forecasts even when a high-dimensional observable space is assumed, and that the Koopman operator can be represented by a sparse matrix.

2 Methodology

2.1 Koopman Operator

The Koopman operator allows linearization of nonlinear dynamical systems. In this case, the dynamics which is nonlinear in a finite dimension, is transformed into an infinite dimensional linear space by introducing observables. For a state variable $y(t)$, consider the following mapping that transfers one observation value to another:

$$\mathcal{K}F(y(t)) = F\left(A(y(t))\right) \tag{1}$$

where $y \in \mathbb{Y}$ is state variable, $\mathbb{Y}$ is finite-dimensional state space, $A : \mathbb{Y} \to \mathbb{Y}$ is nonlinear mapping in state space $\mathbb{Y}$, $F : \mathbb{Y} \to \mathbb{R}$ is nonlinear mapping in the space $\mathcal{F}$ of observables, and $\mathcal{K} : \mathcal{F} \to \mathcal{F}$ is mapping from the space of observables to the space of different observables.

With respect to Eq. (1), the operator that specifically takes into account the time evolution of the state variable is called the Koopman operator. Using the Koopman operator, the time evolution of the time-variant state variable $y(t)$ can be expressed as follows:

$$\mathcal{K}_s F(y(t)) = F(y(t+s)) \tag{2}$$

where t and s are real numbers representing time, and $\mathcal{K}_s$ is the Koopman operator, which is the operator that leads to the s-step forward time evolution. Since the Koopman operator is a linear operator, the following properties of linear operators can be used:

$$\mathcal{K}_s\left\{c_1 f_1(y(t)) + c_2 f_2(y(t))\right\} = c_1 \mathcal{K}_s f_1(y(t)) + c_2 \mathcal{K}_s f_2(y(t)) \tag{3}$$

where $c_1, c_2 \in \mathbb{R}$ and $f_1, f_2 \in \mathcal{F}$.

When performing calculations using the Koopman operator, it is necessary to approximate an infinite-dimensional operator with a finite-dimensional one due to the limitation of computational resources. Therefore it is important to introduce a function space that is compatible with the characteristics of nonlinear dynamical systems for estimation dynamical systems using the Koopman operator.

2.2 Proposed Method

In this paper we propose a method to select a function from a large number of candidate functions by using sparsity, aiming to achieve accuracy in dynamical system estimation with a better approximation of the Koopman operator in finite dimensions. Since the Koopman operator is a linear operator, it can be approximated using matrices as follows:

$$\mathcal{K}_s \approx \left[\boldsymbol{k}_1 \quad \boldsymbol{k}_2 \quad \cdots \quad \boldsymbol{k}_p\right]^\top \in \mathbb{R}^{p\times p} \tag{4}$$

where $p \in \mathbb{Z}$ is the number of observables to define and $\boldsymbol{k}_1, \cdots, \boldsymbol{k}_p \in \mathbb{R}^p$ are elements of the Koopman operator in each row.

Let the observables be $f_1(y(t)), \cdots, f_p(y(t))$, and focusing on $f_i(y(t))$, it can be expressed as follows using the approximation in Eq. (4):

$$f_i(y(t+s)) \approx \sum_{j=1}^{p} k_{i,j} f_j(y(t)) \tag{5}$$

We estimate to be sparse with respect to this coefficient k_i. We consider the following loss function with respect to the coefficients k_i corresponding to all observables($i = 1, ..., p$):

$$\mathcal{L}(\boldsymbol{k}_i) = \left\| f_i(y(t+s)) - \sum_{j=1}^{p} k_{i,j} f_j(y(t)) \right\|_2^2 + \lambda \|\boldsymbol{k}_i\|_1 \tag{6}$$

The sparse coefficients can be estimated by minimizing Eq. (6). By performing this minimization for each observable, the Koopman operator is reconstructed as follows:

$$\mathcal{K}_s^\star \approx \left[\boldsymbol{k}_1^\star \quad \boldsymbol{k}_2^\star \quad \cdots \quad \boldsymbol{k}_p^\star\right]^\top \in \mathbb{R}^{p\times p} \tag{7}$$

Estimated Koopman operator $\mathcal{K}_s^\star$ has smaller values of elements, especially eliminating the effects of unnecessary coefficients. The reproduction of the behavior of the state variable $y(t)$ can be calculated by including $y(t)$ as the observable. Set $f_1(y(t)) = y(t)$ and repeat the following lines of calculation:

$$\left[y(t+s) \quad f_2(y(t+s) \quad \cdots \quad f_p(t+s))\right]^\top = \mathcal{K}_s^\star \left[y(t) \quad f_2(y(t)) \quad \cdots \quad f_p(y(t))\right]^\top \tag{8}$$

By performing this calculation, the observable $f_1(y(t)) = y(t)$ is the value corresponding to the behavior of the system.

3 Results

To evaluate the performance of the proposed method, experimental results are presented for two nonlinear dynamical systems: a single pendulum and a Duffing oscillator. The evaluation criterion is the long-term prediction accuracy when only initial values are given, and the sparsity of the Koopman operator is also evaluated. To demonstrate the superiority of the proposed method, we compare our method with the least squares method without regularization (LSM). The hyperparameter λ of the proposed method was selected to provide the highest long-term forecast accuracy.

3.1 Single Pendulum

In this experiment, we consider the behavior of the state variable of a single pendulum, which is formulated by the following simultaneous differential equations:

$$\frac{\mathrm{d}y_1(t)}{\mathrm{d}t} = \frac{y_2(t)}{m} \tag{9}$$

$$\frac{\mathrm{d}y_2(t)}{\mathrm{d}t} = -mg\sin(y_1(t)) \tag{10}$$

where $y_1(t)$ and $y_2(t)$ are the state variables and m and g are the parameters of the system. For training, data points of time span $0 \leq t \leq 2$ at 0.05 intervals were used. Polynomials up to the 10th order of the state variables $y_1(t)$ and $y_2(t)$ were prepared in advance as the observed values.

The results of the long-term forecasts given only the initial values are shown in Figure 1. LSM shows divergence as early as in the prediction of the next step of the initial value. On the other hand, the proposed method reproduces the behavior quite accurately over a span up to $t = 50$, which is longer than the training data; root mean square error (RMSE) is 2.69×10^{-5}, which quantitatively guarantees the forecast's accuracy.

Next, Figure 2 shows a visualization of the elements of the estimated Koopman operator. It can be seen that the Koopman operator estimated by LSM has large absolute values of its elements. On the other hand, the operator estimated by the proposed method has smaller absolute values than does the operator estimated by LSM. In particular, there are more zero elements: 0.02% (1 element) for LSM and 52.07% (2200 elements) for the proposed method. In the method without regularization, the fitting becomes complicated and positive and negative values tend to cancel each other out. On the other hand, it can be seen that the proposed method achieves the selection

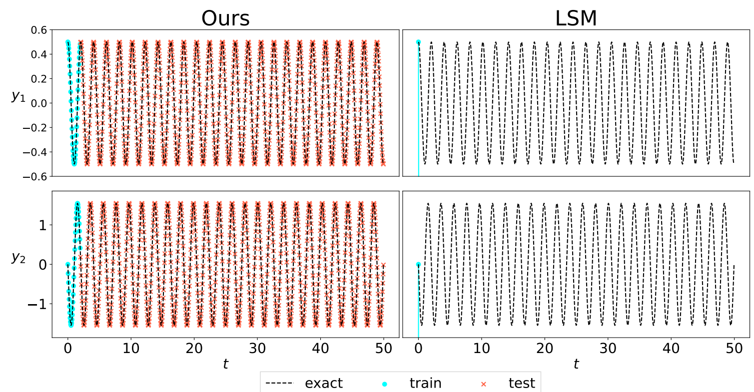

Figure 1: Comparison of long-term forecasts in a single pendulum. True trajectories (black dashed lines) and predictions for the training period (blue dots) and the test period (red crosses) are shown. The results of long-term forecasts by LSM deviate from the true trajectories after the next point of the initial values.

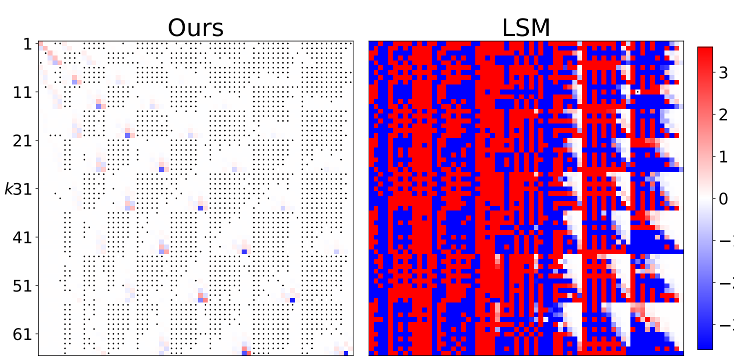

Figure 2: Comparison of estimated Koopman operators in a single pendulum. The operator estimated by the proposed method (left figure) and one estimated by LSM (right figure) are visualized in the form of Eq. (4). As the element increases in the positive direction, the red becomes darker, and as the element moves toward the negative direction, the blue becomes darker. As the element approaches zero, it becomes whiter, and a completely zero element is represented by a black dot.

of observables by imparting sparsity and suppresses the appearance of elements that are unnecessary for reproducing the behavior.

3.2 Duffing Oscillator

The Duffing oscillator formulation is as follows:

$$\frac{\mathrm{d}y_1(t)}{\mathrm{d}t} = y_2(t) \tag{11}$$

$$\frac{\mathrm{d}y_2(t)}{\mathrm{d}t} = -ay_1(t) - by_1^3(t) \tag{12}$$

where $y_1(t), y_2(t)$ are the state variables and a, b are the parameters of the system. For training, data points of time span $0 \leq t \leq 4$ at 0.05 intervals were used. Polynomials up to the 10th order of the state variables $y_1(t)$ and $y_2(t)$ were prepared in advance as the observed values.

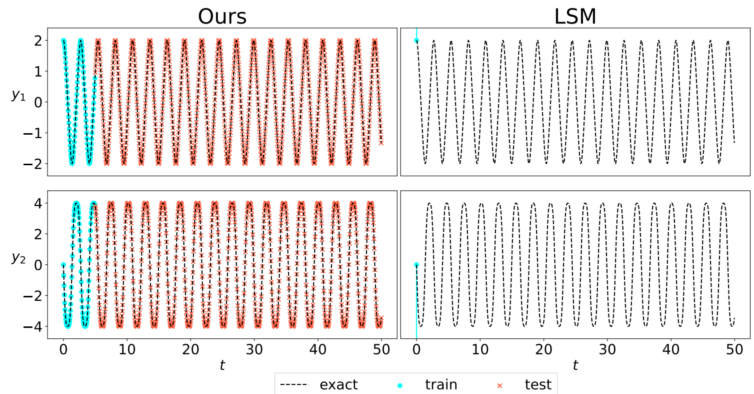

Figure 3: Comparison of long-term forecasts in Duffing oscillator. See the caption for Figure 1.

Figure 3 shows the results of the long-term forecasts given only the initial values As in the case of the single pendulum, the proposed method reproduces the behavior quite accurately for spans up to $t = 50$, which is longer than the training data, while LSM shows divergence at the prediction of the next step of the initial value. RMSE of the long-term forecasts of the proposed method is 8.82×10^{-5}, which assures that the accuracy is quantitatively high.

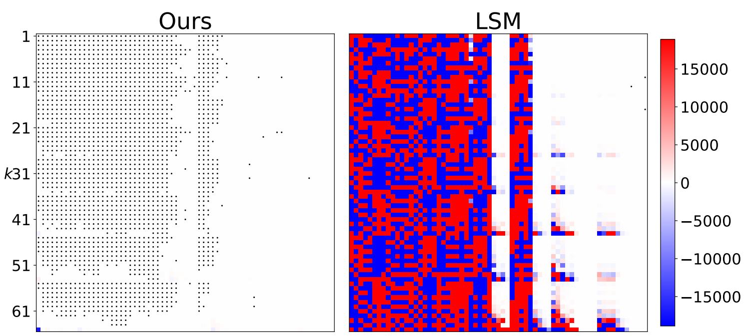

Figure 4: Comparison of estimated Koopman operators in Duffing oscillator. See the caption for Figure 2.

A visualization of the estimated Koopman operators is shown in Figure 4. The Koopman operator estimated by LSM has large absolute values of their elements, while the operator estimated by the proposed method has smaller absolute values than does the operator estimated by LSM. Zero elements also occur more frequently: 0.07% (3 elements) for LSM and 46.84% (1979 elements) for the proposed method. The matrix with more zero elements derived by the proposed method can be applied to algorithms such as sparse matrices, which may lead to a reduction in the computational complexity of the simulation.

4 Conclusion

In this paper we propose a method for estimating dynamical systems using a sparse representation of a Koopman operator. This is a data-driven estimation of the Koopman operator that imposes a constraint on the magnitude of the absolute values of the elements, aiming to appropriately approximate a Koopman operator, which is originally infinite-dimensional, in finite dimensions. In the dynamical system estimation using a Koopman operator, when many functions are assumed as observables, it is shown that the proposed method is considerably superior to the unconstrained method in terms of long-term forecasts. It was also shown that Koopman operators with many zero elements were estimated, and the possibility of applying the method to sparse matrices was also demonstrated.

Acknowledgments

This work was partially supported by Grant-in-Aid for Scientific Research (B) (No. JP21H03509), and a Fund for the Promotion of Joint International Research (International Collaborative Research) (No. JP23KK0184), MEXT, Japan, CREST (No. JPMJCR1914), JST, Japan.

References

[1] Amin G. and Bogdan I. G. Data-driven prediction in dynamical systems: recent developments. *Phil. Trans. R. Soc. A.*, 380:20210213, 2022.

[2] Course K. and Nair P. B. State estimation of a physical system with unknown governing equations. *Nature*, 622(7982):261–267, 2023.

[3] Filoche A., Béréziat D., and Charantonis A. Deep prior in variational assimilation to estimate an ocean circulation without explicit regularization. *Environmental Data Science*, 2:e2, 2023.

[4] Yadav N., Ravela S., and Ganguly A. R. Machine Learning for Robust Identification of Complex Nonlinear Dynamical Systems: Applications to Earth Systems Modeling. *ArXiv*, abs/2008.05590, 2020.

[5] Chattopadhyay A., Hassanzadeh P., and Subramanian D. Data-driven predictions of a multiscale Lorenz 96 chaotic system using machine-learning methods: reservoir computing, artificial neural network, and long short-term memory network. *Nonlinear Processes in Geophysics*, 27(3):373–389, 2020.

[6] Maulik R. Hamzi B. and Owhadi H. Simple, low-cost and accurate data-driven geophysical forecasting with learned kernels. *Proc. R. Soc. A.*, 477:20210326, 2021.

[7] Tandeo P., Aillio P., and Sévellec F. Data-driven reconstruction of partially observed dynamical systems. *Nonlinear Processes in Geophysics*, 30(2):129–137, 2023.

[8] Omori T., Kuwatani T., Okamoto A., and Hukushima K. Bayesian inversion analysis of nonlinear dynamics in surface heterogeneous reactions. *Phys. Rev. E*, 94:033305, 2016.

[9] Oyanagi R., Kuwatani T., and Omori T. Exploration of nonlinear parallel heterogeneous reaction pathways through Bayesian variable selection. *Eur. Phys. J. B*, 94:42, 2021.

[10] Agostini L. Exploration and prediction of fluid dynamical systems using auto-encoder technology. *Physics of Fluids*, 32(6):067103, 2020.

[11] Cheng S., Lucor D., and Argaud J. P. Observation data compression for variational assimilation of dynamical systems. *Journal of Computational Science*, 53:101405, 2021.

[12] Yu C., Bi X., and Fan Y. Deep learning for fluid velocity field estimation: A review. *Ocean Engineering*, 271:113693, 2023.

[13] Jayaraman B. and Mamun S M A. A. On Data-Driven Sparse Sensing and Linear Estimation of Fluid Flows. *Sensors*, 20(13), 2020.

[14] Sholahudin, Giannetti N., Yamaguchi S., Saito K., Miyaoka Y., Tanaka K., and Ogami H. Experimental implementation of artificial neural network for cost effective and non-intrusive performance estimation of air conditioning systems. *Applied Thermal Engineering*, 181:115985, 2020.

[15] Alonso-Bastida A., Franco-Nava M. A., Adam-Medina M., López-Zapata B., Álvarez Gutiérrez P. E., and García-Morales J. Mathematical modeling of thermal interactions in a self-cooling pilot-scale photobioreactor. *Case Studies in Thermal Engineering*, 31:101825, 2022.

[16] Brunton S. L., Budišić M., Kaiser E., and Nathan Kutz J. Modern Koopman Theory for Dynamical Systems. *SIAM Rev.*, 64:229–340, 2021.

[17] Otto S. E. and Rowley C. W. Koopman Operators for Estimation and Control of Dynamical Systems. *Annual Review of Control, Robotics, and Autonomous Systems*, 4(1):59–87, 2021.

[18] Kostic V., Novelli P., Maurer A., Ciliberto C., Rosasco L., and Pontil M. Learning Dynamical Systems via Koopman Operator Regression in Reproducing Kernel Hilbert Spaces. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh, editors, *Advances in Neural Information Processing Systems*, volume 35, pages 4017–4031. Curran Associates, Inc., 2022.

[19] Narendra K. S. and Parthasarathy K. Neural networks and dynamical systems. *International Journal of Approximate Reasoning*, 6(2):109–131, 1992.

[20] Bevanda P., Sosnowski S., and Hirche S. Koopman operator dynamical models: Learning, analysis and control. *Annual Reviews in Control*, 52:197–212, 2021.

[21] Kaiser E., Kutz J. N., and Brunton S. L. Data-driven discovery of Koopman eigenfunctions for control. *Machine Learning: Science and Technology*, 2(3):035023, 2021.

[22] Li M. and Jiang L. Deep learning nonlinear multiscale dynamic problems using Koopman operator. *Journal of Computational Physics*, 446:110660, 2021.

[23] Korda M., Putinar M., and Mezić I. Data-driven spectral analysis of the Koopman operator. *Applied and Computational Harmonic Analysis*, 48(2):599–629, 2020.