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Optimal Model Selection for Estimating Stochastic Koopman Modes

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Abstract—Dynamic mode decomposition (DMD) is a method of modal extraction from time series data, which models the latent nonlinear dynamics underlying the data in terms of the dynamical systems theory. Recently, the extended DMD (EDMD) [M. Williams et al., 2015], which significantly widens the applicability of DMD, has been proposed. However, selecting an optimal setting of EDMD for given data is still an open question. In this study, we propose an algorithm to select the optimal hyperparameter of EDMD. The validity of our method is demonstrated by numerical experiments.

1. Introduction

EDMD [2] extends the original DMD [1] by mapping time series data into a high-dimensional feature space, and enables the application of DMD to a broader class of nonlinear dynamical systems. However, the optimal hyperparameter selection of EDMD is not straightforward, because the feature space of EDMD cannot be selected by the ordinary cross validation. In this study, we propose an approximate cross validation algorithm to select the optimal hyperparameter of EDMD for each mode, which improves the robustness and applicability of EDMD.

2. Koopman theory and DMD

DMD is mathematically formulated by using a linear operator, called the Koopman operator, that describes the temporal evolution of time series. For a dynamical system $\boldsymbol{x}_{t+1} \sim p(\cdot|\boldsymbol{x}_t)$, the corresponding Koopman operator $\mathcal{K}$ is defined as an expectation operator as follows:

$$(\mathcal{K}f)(\boldsymbol{x}) = \int f(\boldsymbol{x}')p(\boldsymbol{x}'|\boldsymbol{x})d\boldsymbol{x}'. \qquad (1)$$

If $\mathcal{K}$ has point spectra, one can define the eigenpairs $\{(\lambda_j, \xi_j(\boldsymbol{x}))\}$ of $\mathcal{K}$ satisfying the following relation:

$$(\mathcal{K}\xi_j)(\boldsymbol{x}) = \lambda_j \xi_j(\boldsymbol{x}). \qquad (2)$$

DMD and EDMD compute the eigenpairs for modal extraction. Thus, it is necessary to select the optimal hyperparameter that minimizes the estimation error of the eigenpairs.

3. Proposed method

To select the optimal hyperparameter for each mode, we repeatedly compute candidate estimates of eigenpairs by EDMD with different candidate hyperparameters, classify the candidate eigenpairs into groups corresponding to the same true eigenpairs, and select the optimal eigenpair in each group. Let Θ be a hyperparameter set representing the setting of EDMD, e.g., a kernel function, kernel parameters, and regularization parameters. For a given time series $\{\boldsymbol{x}_t\}_{t=1,2,...}$ and given candidate hyperparameter sets $\{\Theta_\ell\}_{\ell=1,2,...}$, one can select the optimal hyperparameter set for estimating each true eigenpair as follows:

1. For each hyperparameter set Θ_ℓ, apply EDMD to the dataset $\{\boldsymbol{x}_t\}_{t=1,2,...}$. Let $(\lambda_k^{(\ell)}, \xi_k^{(\ell)}(\boldsymbol{x}))$ be the k-th eigenvalue and eigenfunction computed with Θ_ℓ, which we call the (k, ℓ)-th candidate eigenpair.

2. Apply the single-linkage hierarchical clustering algorithm to all the eigenpairs $\{(\lambda_k^{(\ell)}, \xi_k^{(\ell)}(\boldsymbol{x}))\}_{k,\ell=1,2,...}$. The distance between the (k, ℓ)-th and (k', ℓ')-th eigenpairs is defined as $1 - (C_{k\ell k'\ell'} + C_{k'\ell' k\ell})/2$, where $C_{k\ell k'\ell'}$ is the cosine distance between the time series of the Koopman and Perron-Frobenius eigenfunctions of the (k, ℓ)-th and (k', ℓ')-th eigenpairs, respectively. Let C_j be the set of the eigenpairs $(\lambda_k^{(\ell)}, \xi_k^{(\ell)}(\boldsymbol{x}))$ belonging to the j-th cluster.

3. For each cluster C_j, apply the m-fold cross validation to the all eigenpairs in C_j for selecting the optimal eigenpair $(\lambda^*, \xi^*(\boldsymbol{x})) \in C_j$ that minimizes the cross validation error $\sum_t |\xi^*(\boldsymbol{x}_{t+1}) - \lambda^*\xi^*(\boldsymbol{x}_t)|^2 / \sum_t |\xi^*(\boldsymbol{x}_t)|^2$.

Since the Koopman and Perron-Frobenius eigenfunctions form a biorthogonal system, each cluster C_j is expected to include candidate estimates of the same true eigenpair. Thus, one can select the optimal hyperparameter set and eigenpair estimate for each true eigenpair.

References

[1] P. J. Schmid, J. Fluid Mech. 656 (2010): 5-28.

[2] M. Williams, C. W. Rowley, and I. G. Kevrekidis, J. Nonlin. Sci. (2015); J. Comput. Dyn. (2015).