PyKoopman: A Python Package for Data-Driven Approximation of the Koopman Operator

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Summary

`PyKoopman` is a Python package for the data-driven approximation of the Koopman operator associated with a dynamical systems. The Koopman operator is a principled linear embedding of nonlinear dynamics and facilitates the prediction, estimation, and control of strongly nonlinear dynamics using linear systems theory. In particular, `PyKoopman` provides tools for data-driven system identification for unforced and actuated systems that build on the equation-free dynamic mode decomposition (DMD) (Schmid 2010) and its variants (Kutz et al. 2016; Schmid 2022; Brunton et al. 2022). In this work, we provide a brief description of the mathematical underpinnings of the Koopman operator, an overview and demonstration of the features implemented in `PyKoopman` (with code examples), practical advice for users, and a list of potential extensions to `PyKoopman`. Software is available at https://github.com/dynamicslab/pyKoopman.

Statement of need

Engineers have long relied on linearization to bridge the gap between simplified, descriptions where powerful analytical tools exist, and the intricate complexities of nonlinear dynamics where analytical solutions are elusive (Ljung 2010; Wright, Nocedal, and others 1999). Local linearization, implemented via first-order Taylor series approximation, has been widely used in system identification (Ljung 2010), optimization (Wright, Nocedal, and others 1999), and many other fields to make problems tractable. However, many real-world systems are fundamentally nonlinear and require solutions outside of the local neighborhood where linearization is valid. Rapid progress in machine learning and big data methods are driving advances in the data-driven modeling of such nonlinear systems in science and engineering (Brunton and Kutz 2022). As shown in Fig. 1, Koopman operator theory in particular is a principled approach to embed nonlinear dynamics in a linear framework that goes beyond simple linearization (Brunton et al. 2022).

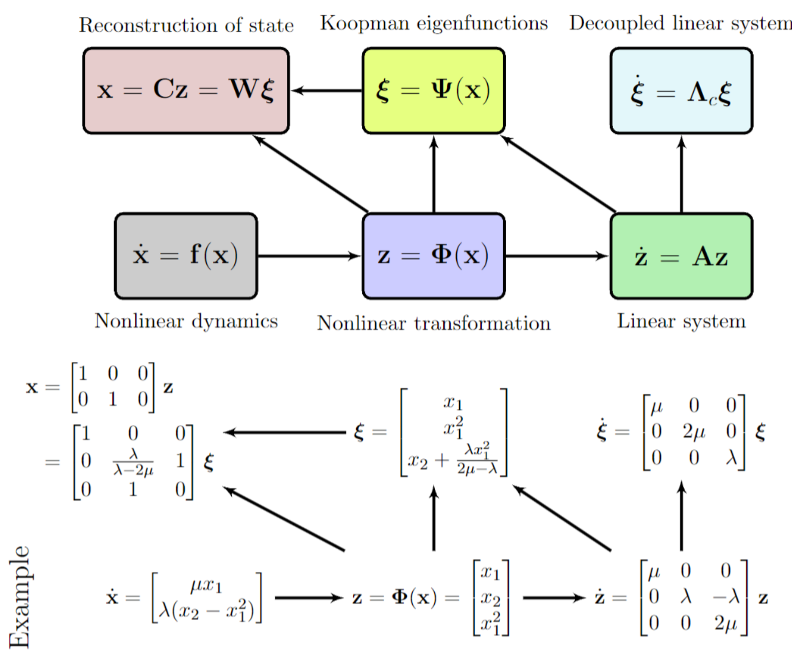

Figure 1: Lifting of the state $\mathbf{x}$ of the continuous autonomous dynamical system into a new coordinate system, in which the original nonlinear dynamics become linear and are easier to handle. One can also linearly reconstruct the state $\mathbf{x}$ from the new coordinate system. This is facilitated with `PyKoopman` in a data-driven manner.

In the diverse landscape of data-driven modeling approaches, Koopman operator theory has received considerable attention in recent years (Budišić, Mohr, and Mezić 2012; Mezić 2013; Williams, Kevrekidis, and Rowley 2015; Klus et al. 2018; Li et al. 2017; Brunton et al. 2017). These strategies encompass not only linear methodologies (Nelles 2020; Ljung 2010) and dynamic mode decomposition (DMD) (Schmid 2010; Rowley et al. 2009; Kutz et al. 2016), but also more advanced techniques such as nonlinear autoregressive algorithms (Akaike 1969; Billings 2013), neural networks (Long et al. 2018; Yang, Zhang, and Karniadakis 2020; Wehmeyer and Noé 2018; Mardt et al. 2018; Vlachas et al. 2018; Pathak et al. 2018; Lu et al. 2021; Raissi, Perdikaris, and Karniadakis 2019; Champion et al. 2019; Raissi, Yazdani, and Karniadakis 2020), Gaussian process regression (Raissi, Babaee, and Karniadakis 2019), operator inference, and reduced-order modeling (Benner, Gugercin, and Willcox 2015, @peherstorfer2016data, @qian2020lift), among others (Giannakis and Majda 2012; Yair et al. 2017; Bongard and Lipson 2007; Schmidt and Lipson 2009; Daniels and Nemenman 2015; Brunton, Proctor, and Kutz 2016; Rudy et al. 2017). The Koopman operator perspective is unique within data-driven modeling techniques due to its distinct aim of learning a coordinate system in which the nonlinear dynamics become linear. This methodology enables the application of closed-form, convergence-guaranteed methods from linear system theory to general nonlinear dynamics. To fully leverage the potential of data-driven Koopman theory across a diverse range of scientific and engineering disciplines, it is critical to have a central toolkit to automate state-of-the-art Koopman operator algorithms.

As a result, the `PyKoopman` is developed as a Python package for approximating the Koopman operator associated with natural and actuated dynamical systems from measurement data. Compared to implementation of DMD (e.g., `PyDMD` (Demo, Tezzele, and Rozza 2018)) which can be viewed as a linear projection of Koopman operator, `PyKoopman` offers a comprehensive set of *nonlinear* projection methods (e.g., polynomial basis or kernel trick, neural network (Pan and Duraisamy 2020)) together with sparsity promoting algorithms for *nonlinear* projection methods optimal modes selection (Pan, Arnold-Medabalimi, and Duraisamy 2021). Specifically, `PyKoopman` offers tools for designing the observables (i.e., functions of the system state) and inferring a finite-dimensional linear operator that governs the dynamic evolution of these observables in time. These steps can either be performed sequentially (Williams, Rowley, and Kevrekidis 2015; Williams, Kevrekidis, and Rowley 2015) or combined, as demonstrated in more recent neural network models (Lusch, Kutz, and Brunton 2018; Otto and Rowley 2019; Mardt et al. 2018; Takeishi, Kawahara, and Yairi 2017). Besides, we also support data from multiple trajectories. Once a linear embedding is discovered from the data, the linearity of the transformed dynamical system can be leveraged for enhanced interpretability (Pan, Arnold-Medabalimi, and Duraisamy 2021) or for designing near-optimal observers (Surana and Banaszuk 2016) or controllers for the original nonlinear system (Korda and Mezić 2020; Mauroy, Susuki, and Mezić 2020; Kaiser, Kutz, and Brunton 2021; Peitz and Klus 2019; Peitz, Otto, and Rowley 2020).

Features

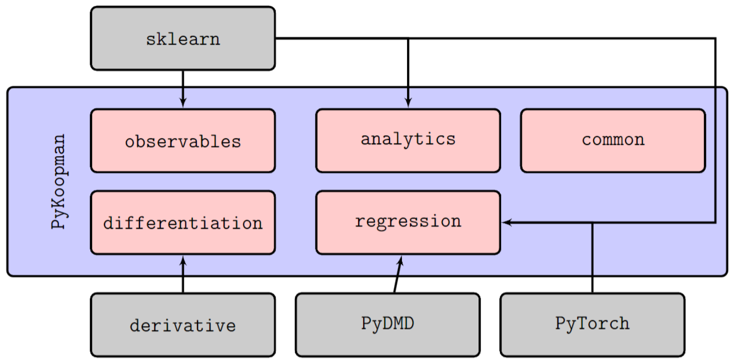

Figure 2: External package dependencies of PyKoopman.

The core component of the PyKoopman package is the Koopman model class. The external package dependencies are depicted in Fig. 2. Below are justifications for each dependency:

- `sklearn`: Scikit-learn is an open-source machine learning library that supports various functionalities throughout the standard machine learning pipeline, including learning algorithms, data preprocessing, model evaluation, and model selection. Firstly, as a standard, user-friendly infrastructure for machine learning, integrating sklearn ensures that our `pykoopman` package reaches a wider audience. Secondly, common utilities (e.g., kernel functions) from sklearn facilitate the abstraction of kernel-based methods. Consequently, the classes within `pykoopman`.regression are implemented as scikit-learn estimators, specifically, sklearn.base.BaseEstimator. Moreover, users can create intricate pipelines for hyperparameter tuning and model selection by synergizing `pykoopman` with scikit-learn.
- `torch`: Relying solely on sklearn restricts us from developing more versatile and advanced algorithms for the Koopman operator. Thus, we have implemented neural network-based methods using PyTorch ('torch" (Paszke et al. 2019)), an open-source library tailored for neural network-based deep learning models, all the while adhering to the sklearn framework. Additionally, we incorporate lightning to streamline the process for users to leverage local AI accelerators (e.g., GPU, TPU) without delving into intricate implementation details.
- `pydmd`: PyDMD (`pydmd` (Demo, Tezzele, and Rozza 2018)) is a Python package crafted for DMD. As many Koopman algorithms mirror DMD steps, it's advantageous to repurpose existing implementations. However, PyDMD supports data predominantly in the form of single trajectories, typical in fluid dynamics, and not uniform samples in phase space or multiple trajectories, which are more prevalent in robotics. To cater to

both sectors, we have extended support beyond single trajectories while also integrating the use of pydmd within `pykoopman`.

- `derivative`: The ‘derivative“ package (Kaptanoglu et al. 2022) is tailored for differentiating noisy data in Python. We utilize this package to discern the Koopman generator from data.

As illustrated in Fig. 3, `PyKoopman` is designed to lift nonlinear dynamics into a linear system with linear actuation. Specifically, our `PyKoopman` implementation involves two major steps:

Unforced

$$\mathbf{z}_{k+1} = \mathbf{A}\mathbf{z}_k$$

Controlled

$$\begin{bmatrix} \mathbf{z} \\ \mathbf{u} \end{bmatrix}_{k+1} = \underbrace{\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \cdot & \cdot \end{bmatrix}}_{=\mathbf{K}} \begin{bmatrix} \mathbf{z} \\ \mathbf{u} \end{bmatrix}_k$$

Figure 3: {Broad categorization of model types that can be identified with current `PyKoopman`. While the dotted parts (marked with “$\cdot$’ ’) can be simultaneously discovered within the framework, they are typically ignored for control purposes.

- `observables`: the nonlinear observables used to lift $\mathbf{x}$ to $\mathbf{z}$, and reconstruct $\mathbf{x}$ from $\mathbf{z}$;
- `regression`: the regression used to find the optimal $\mathbf{A}$.

Additionally, we have a `differentiation` module that evaluates the time derivative from a trajectory and the `analytics` module for sparsifying arbitrary approximations of the Koopman operator.

At the time of writing, we have the following features implemented:

- Observable library for lifting the state $\mathbf{x}$ into the observable space
  - Identity (for DMD/DMDc or in case users want to compute observables themselves): `Identity`
  - Multivariate polynomials: `Polynomial` (Williams, Kevrekidis, and Rowley 2015)
  - Time delay coordinates: `TimeDelay` (Mezić and Banaszuk 2004; Brunton et al. 2017)
  - Radial basis functions: `RadialBasisFunctions` (Williams, Kevrekidis, and Rowley 2015)
  - Random Fourier features: `RandomFourierFeatures` (DeGennaro and Urban 2019)
  - Custom library (defined by user-supplied functions): `CustomObservables`

  - Concatenation of observables: `ConcatObservables`

- System identification method for performing regression
  - Dynamic mode decomposition (Schmid 2010; Rowley et al. 2009): `PyDMDRegressor`
  - Dynamic mode decomposition with control (Proctor, Brunton, and Kutz 2016): `DMDc`
  - Extended dynamic mode decomposition (Williams, Kevrekidis, and Rowley 2015): `EDMD`
  - Extended dynamic mode decomposition with control (Korda and Mezić 2020): `EDMDc`
  - Kernel dynamic mode decomposition (Williams, Rowley, and Kevrekidis 2015): `KDMD`
  - Hankel DMD (Brunton, Proctor, and Kutz 2016): `HDMD`
  - Hankel DMD with control: `HDMDc`
  - Neural Network DMD (Pan and Duraisamy 2020; Otto and Rowley 2019; Lusch, Kutz, and Brunton 2018): `NNDMD`

- Sparse construction of Koopman invariant subspace
  - Multi-task learning based on linearity consistency (Pan, Arnold-Medabalimi, and Duraisamy 2021): `ModesSelectionPAD21`

- Numerical differentiation for computing $\dot{\mathbf{X}}$ from $\mathbf{X}$
  - Finite difference: `FiniteDifference`
  - 4th order central finite difference: `Derivative(kind="finite_difference")`
  - Savitzky-Golay with cubic polynomials: `Derivative(kind="savitzky-golay")`
  - Spectral derivative: `Derivative(kind="spectral")`
  - Spline derivative: `Derivative(kind="spline")`
  - Regularized total variation derivative: `Derivative(kind="trend_filtered")`

- Common toy dynamics
  - Discrete-time random, stable, linear state-space model: `drss`
  - Van del Pol oscillator: `vdp_osc`
  - Lorenz system: `lorenz`
  - Two-dimensional linear dynamics: `Linear2Ddynamics`
  - Linear dynamics on a torus: `torus_dynamics`
  - Forced Duffing Oscillator: `forced_duffing`
  - Cubic-quintic Ginzburg-Landau equation: `cqgle`
  - Kuramoto-Sivashinsky equation:`ks`
  - Nonlinear Schrodinger equation: `nls`
  - Viscous Burgers equation: `vbe`

- Validation routines for consistency checks

Conclusion

Our goal of the `PyKoopman` package is to provide a central hub for education, application and research development of learning algorithms for Koopman operator. The `PyKoopman` package is aimed at researchers and practitioners alike, enabling anyone with access to discover linear embeddings of nonlinear systems from data. Following `PySINDy` (Silva et al. 2020) and `Deeptime` (Hoffmann et al. 2021), `PyKoopman` is designed to be accessible to users with basic knowledge of linear systems, adhering to `scikit-learn` standards, while also being modular for more advanced users. We hope that researchers and practioners will use `PyKoopman` as a platform for algorithms developement and applications of linear embedding.

Acknowledgments

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