PySensors: A Python package for sparse sensor placement

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Extra material added in by Brian

What should the paper contain?

From the JOSS submission guide:

"JOSS welcomes submissions from broadly diverse research areas. For this reason, we require that authors include in the paper some sentences that explain the software functionality and domain of use to a non-specialist reader. We also require that authors explain the research applications of the software. The paper should be between 250-1000 words.

Your paper should include:

- A list of the authors of the software and their affiliations, using the correct format (see the example below).
- A summary describing the high-level functionality and purpose of the software for a diverse, non-specialist audience.
- A clear Statement of Need that illustrates the research purpose of the software.
- A list of key references, including to other software addressing related needs
- Mention (if applicable) a representative set of past or ongoing research projects using the software and recent scholarly publications enabled by it.
- Acknowledgement of any financial support."

See also the review checklist to get an idea of what the reviewers are looking for.

Compiling this document

Make sure you have pandoc installed.

pandoc -s --bibliography paper.bib --filter pandoc-citeproc paper.md -o paper.pdf

Code

You can include code as follows

```
def fib(n):
if n < 2:
    return n
else:
    return fib(n - 1) + fib(n - 2)</pre>
```

Other examples

Here are some other example JOSS papers:

- Example on JOSS website
- pyomeca this one is a bit long, but shows how figures can be incorporated into a JOSS submission
- All published papers

Summary

Scientists have long quantified empirical observations by developing mathematical models that characterize the observations, have some measure of interpretability, and are capable of making predictions. Dynamical systems models in particular have been widely used to study, explain, and predict system behavior in a wide range of application areas, with examples ranging from Newton's laws of classical mechanics to the Michaelis-Menten kinetics for modeling enzyme kinetics. While governing laws and equations were traditionally derived by hand, the current growth of available measurement data and resulting emphasis on data-driven modeling motivates algorithmic approaches for model discovery. A number of such approaches have been developed in recent years and have generated widespread interest, including Eureqa (Schmidt and Lipson 2009), sure independence screening and sparsifying operator (Ouvang et al. 2018), and the sparse identification of nonlinear dynamics (SINDy) (Brunton, Proctor, and Kutz 2016). Maximizing the impact of these model discovery methods requires tools to make them widely accessible to scientists across domains and at various levels of mathematical expertise.

PySINDy is a Python package for the discovery of governing dynamical systems models from data. In particular, PySINDy provides tools for applying the SINDy approach to model discovery (Brunton, Proctor, and Kutz 2016). Given data in the form of state measurements $\mathbf{x}(t) \in \mathbb{R}^n$, the SINDy method seeks a function \mathbf{f} such that

$$\frac{d}{dt}\mathbf{x}(t) = \mathbf{f}(\mathbf{x}(t)).$$

SINDy poses this model discovery as a sparse regression problem, wherein relevant terms in \mathbf{f} are selected from a library of candidate functions. Thus,

SINDy models balance accuracy and efficiency, resulting in parsimonious models that avoid overfitting while remaining interpretable and generalizable. This approach is straightforward to understand and can be readily customized using different sparse regression algorithms or library functions.

The PySINDy package is aimed at researchers and practitioners alike, enabling anyone with access to measurement data to engage in scientific model discovery. The package is designed to be accessible to inexperienced practitioners, while also including options that allow more advanced users to customize it to their needs. A number of popular SINDy variants are implemented, but PySINDy is also designed to enable further extensions for research and experimentation. The package follows object-oriented design and is scikit-learn compatible.

The SINDy method has been widely applied for model identification in applications such as chemical reaction dynamics (Hoffmann, Fröhner, and Noé 2019), nonlinear optics (Sorokina, Sygletos, and Turitsyn 2016), thermal fluids (Loiseau 2019), plasma convection (Dam et al. 2017), numerical algorithms (Thaler, Paehler, and Adams 2019), and structural modeling (Lai and Nagarajaiah 2019). It has also been extended to handle more complex modeling scenarios such as partial differential equations (Schaeffer 2017; Rudy et al. 2017), systems with inputs or control (Kaiser, Kutz, and Brunton 2018), corrupt or limited data (Tran and Ward 2017; Schaeffer, Tran, and Ward 2018), integral formulations (Schaeffer and McCalla 2017; Reinbold, Gurevich, and Grigoriev 2020), physical constraints (Loiseau and Brunton 2018), tensor representations (Gelß et al. 2019), and stochastic systems (Boninsegna, Nüske, and Clementi 2018). However, there is not a definitive standard implementation or package for applying SINDy. Versions of SINDy have been implemented within larger projects such as sparsereg (Quade 2018), but no specific implementation has emerged as the most widely adopted and most versions implement only a limited set of features. Researchers have thus typically written their own implementations, resulting in duplicated effort and a lack of standardization. This not only makes it more difficult to apply SINDy to scientific data sets, but also makes it more challenging to benchmark extensions to the method against the original and makes such extensions less accessible to end users. The PySINDy package provides a dedicated central codebase where many of the basic SINDy features are implemented, allowing for easy use and standardization. This also makes it straightforward for users to extend the package in a way such that new developments are available to a wider user base.

Features

The core object in the PySINDy package is the SINDy model class, which is implemented as a scikit-learn estimator. This design was chosen to make the package simple to use for a wide user base, as many potential users will be familiar with scikit-learn. It also expresses the SINDy model object at the appropriate level of abstraction so that users can embed it into more complicated pipelines

in scikit-learn, such as tools for parameter tuning and model selection.

Applying SINDy involves making several modeling decisions, namely: which numerical differentiation method is used, which functions make up the feature library, and which sparse regression algorithm is applied to learn the model. The core SINDy object uses a set of default options but can be easily customized using a number of common approaches implemented in PySINDy. The package provides a few standard options for numerical differentiation (finite difference and smoothed finite difference), feature libraries (polynomial and Fourier libraries, as well as a class for creating custom libraries), and sparse regression techniques (sequentially thresholded least squares (Brunton, Proctor, and Kutz 2016), LASSO (Tibshirani 1996), and sparse relaxed regularized regression (Zheng et al. 2018)). Users can also create their own differentiation, sparse regression, or feature library objects for further customization.

The software package includes tutorials in the form of Jupyter notebooks. These tutorials demonstrate the usage of various features in the package and reproduce the examples from the original SINDy paper (Brunton, Proctor, and Kutz 2016).

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References

- Boninsegna, Lorenzo, Feliks Nüske, and Cecilia Clementi. 2018. "Sparse Learning of Stochastic Dynamical Equations." *The Journal of Chemical Physics* 148 (24): 241723. https://doi.org/10.1063/1.5018409.
- Brunton, Steven L., Joshua L. Proctor, and J. Nathan Kutz. 2016. "Discovering Governing Equations from Data by Sparse Identification of Nonlinear Dynamical Systems." *Proceedings of the National Academy of Sciences* 113 (15): 3932–7. https://doi.org/10.1073/pnas.1517384113.
- Dam, Magnus, Morten Brøns, Jens Juul Rasmussen, Volker Naulin, and Jan S. Hesthaven. 2017. "Sparse Identification of a Predator-Prey System from Simulation Data of a Convection Model." *Physics of Plasmas* 24 (2): 022310. https://doi.org/10.1063/1.4977057.
- Gelß, Patrick, Stefan Klus, Jens Eisert, and Christof Schütte. 2019. "Multidimensional Approximation of Nonlinear Dynamical Systems." Journal of Compusional Approximation of Nonlinear Dynamical Systems."

- tational and Nonlinear Dynamics 14 (6). https://doi.org/10.1115/1.4043148.
- Hoffmann, Moritz, Christoph Fröhner, and Frank Noé. 2019. "Reactive SINDy: Discovering Governing Reactions from Concentration Data." *Journal of Chemical Physics* 150 (025101). https://doi.org/10.1063/1.5066099.
- Kaiser, Eurika, J Nathan Kutz, and Steven L Brunton. 2018. "Sparse Identification of Nonlinear Dynamics for Model Predictive Control in the Low-Data Limit." *Proceedings of the Royal Society of London A* 474 (2219). https://doi.org/10.1098/rspa.2018.0335.
- Lai, Zhilu, and Satish Nagarajaiah. 2019. "Sparse Structural System Identification Method for Nonlinear Dynamic Systems with Hysteresis/Inelastic Behavior." *Mechanical Systems and Signal Processing* 117: 813–42. https://doi.org/10.1016/j.ymssp.2018.08.033.
- Loiseau, J.-C., and Steven L. Brunton. 2018. "Constrained Sparse Galerkin Regression." *Journal of Fluid Mechanics* 838: 42–67. https://doi.org/10.1017/jfm.2017.823.
- Loiseau, Jean-Christophe. 2019. "Data-Driven Modeling of the Chaotic Thermal Convection in an Annular Thermosyphon." arXiv Preprint arXiv:1911.07920.
- Ouyang, Runhai, Stefano Curtarolo, Emre Ahmetcik, Matthias Scheffler, and Luca M. Ghiringhelli. 2018. "SISSO: A Compressed-Sensing Method for Identifying the Best Low-Dimensional Descriptor in an Immensity of Offered Candidates." *Physical Review Materials* 2 (8): 083802. https://doi.org/10.1103/physrevmaterials.2.083802.
- Quade, Markus. 2018. "Sparsereg Collection of Modern Sparse Regression Algorithms." https://doi.org/10.5281/zenodo.1173754.
- Reinbold, Patrick AK, Daniel R Gurevich, and Roman O Grigoriev. 2020. "Using Noisy or Incomplete Data to Discover Models of Spatiotemporal Dynamics." *Physical Review E* 101 (1): 010203. https://doi.org/10.1103/physreve.101.0 10203.
- Rudy, Samuel H, Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz. 2017. "Data-Driven Discovery of Partial Differential Equations." *Science Advances* 3 (e1602614). https://doi.org/10.1126/sciadv.1602614.
- Schaeffer, Hayden. 2017. "Learning Partial Differential Equations via Data Discovery and Sparse Optimization." In *Proceedings of the Royal Society a*, 473:20160446. 2197. The Royal Society. https://doi.org/10.1098/rspa.2016.0446.
- Schaeffer, Hayden, and Scott G McCalla. 2017. "Sparse Model Selection via Integral Terms." *Physical Review E* 96 (2): 023302. https://doi.org/10.1103/physreve.96.023302.
- Schaeffer, Hayden, Giang Tran, and Rachel Ward. 2018. "Extracting Sparse High-Dimensional Dynamics from Limited Data." SIAM Journal on Applied

- Mathematics 78 (6): 3279-95. https://doi.org/10.1137/18m116798x.
- Schmidt, Michael, and Hod Lipson. 2009. "Distilling Free-Form Natural Laws from Experimental Data." *Science* 324 (5923): 81–85. https://doi.org/10.1126/science.1165893.
- Sorokina, Mariia, Stylianos Sygletos, and Sergei Turitsyn. 2016. "Sparse Identification for Nonlinear Optical Communication Systems: SINO Method." Optics Express 24 (26): 30433–43. https://doi.org/10.1364/oe.24.030433.
- Thaler, Stephan, Ludger Paehler, and Nikolaus A Adams. 2019. "Sparse Identification of Truncation Errors." *Journal of Computational Physics* 397: 108851. https://doi.org/10.1016/j.jcp.2019.07.049.
- Tibshirani, Robert. 1996. "Regression Shrinkage and Selection via the Lasso." Journal of the Royal Statistical Society. Series B (Methodological) 58 (1): 267–88. https://doi.org/10.1111/j.2517-6161.1996.tb02080.x.
- Tran, Giang, and Rachel Ward. 2017. "Exact Recovery of Chaotic Systems from Highly Corrupted Data." *Multiscale Modeling & Simulation* 15 (3): 1108–29. https://doi.org/10.1137/16m1086637.
- Zheng, Peng, Travis Askham, Steven L. Brunton, J. Nathan Kutz, and Aleksandr Y. Aravkin. 2018. "A Unified Framework for Sparse Relaxed Regularized Regression: SR3." *IEEE Access* 7: 1404–23. https://doi.org/10.1109/access.2018.2886528.