PySensors: A Python package for sparse sensor placement

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Extra material added in by Brian

TODO: remove extra material

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.
- Acknowledgment 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

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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 (Ouyang et al. 2018), and the sparse identification of nonlinear dynamics (SINDy) (S. L. 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 (S. L. 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 PySensors package can be used by both researchers looking to advance the state of the art and practitioners seeking simple sparse sensor selection methods for their applications of interest. Simple methods and abundant examples help new users to hit the ground running. At the same time modular classes leave flexibility for users to experiment with and plug in new sensor selection algorithms or dimensionality reduction techniques. Users of scikit-learn will find Pysensors syntax familiar and intuitive. The package is fully compatible with scikit-learn and follows object-oriented design principles.

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

PySensors enables the sparse placement of sensors for two classes of problems: reconstruction and classification. For reconstruction problems the package im-

plements a unified SensorSelector class, with methods for efficiently analyzing the effects data or sensor quantity have on reconstruction performance. Often different sensor locations impose variable costs, e.g. if measuring sea-surface temperature, it may be more expensive to place buoys/sensors in the middle of the ocean than close to shore. These costs can be taken into account during sensor selection via a built-in cost-sensitive optimization routine (Clark et al. 2018). For classification tasks, the package implements the Sparse Sensor Placement Optimization for Classification (SSPOC) algorithm (B. W. Brunton et al. 2016), allowing one to optimize sensor placement for classification accuracy. This SSPOC implementation is fully general in the sense that it can be used in conjunction with any linear classifier. Additionally, PySensors provides methods to enable straightforward exploration of the impacts of primary hyperparameters.

It is well known (Manohar et al. 2018) that the basis in which one represents measurement data can have a pronounced effect on the sensors that are selected and the quality of the reconstruction. Users can readily switch between different bases typically employed for sparse sensor selection, including PCA modes and random projections. Because PySensors was built with scikit-learn compatibility in mind, it is easy to use cross-validation to select among possible choices of bases, basis modes, and other hyperparameters.

Finally, included with PySensors is a large suite of examples, implemented as Jupyter notebooks. Some of the examples are written in a tutorial format and introduce new users to the objects, methods, and syntax of the package. Other examples demonstrate intermediate-level concepts such as how to visualize model parameters and performance, how to combine scikit-learn and PySensors objects, selecting appropriate parameter values via cross-validation, and other best-practices. Further notebooks use PySensors to solve challenging real-world problems. The notebooks reproduce many of the examples from the papers upon which the package is based (Manohar et al. 2018; Clark et al. 2018; B. W. Brunton et al. 2016). To help users begin applying PySensors to their own datasets even faster, interactive versions of every notebook are available on Binder. Overall, the examples will compress the learning curve of learning a new software package.

Acknowledgments

TODO: write acknowledgments section

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