

# PyNumDiff: A Python package for numerical differentiation of noisy time-series data

Floris Van Breugel<sup>\*1</sup>, Yuying Liu<sup>2</sup>, Bingni W. Brunton<sup>3</sup>, and J. Nathan Kutz<sup>2</sup>

<sup>1</sup> Department of Mechanical Engineering, University of Nevada at Reno <sup>2</sup> Department of Applied Mathematics, University of Washington <sup>3</sup> Department of Biology, University of Washington

DOI: [10.21105/joss.03922](https://doi.org/10.21105/joss.03922)

## Software

- [Review](#) ↗
- [Repository](#) ↗
- [Archive](#) ↗

Editor: [Christina Hedges](#) ↗

Submitted: 15 November 2021

Published: 19 November 2021

## License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

## Statement of need

The numerical computation of derivatives is ubiquitous in every scientific discipline and engineering application because derivatives express fundamental relationships among many quantities of interest. As a result, a large number of diverse algorithms have been developed to differentiate numerical data. These efforts are challenging because, in reality, practitioners often have sparse and noisy measurements and data, which undermine the ability to estimate accurate derivatives. Among the diversity of mathematical approaches that have been formulated, many are ad hoc in nature and require significant bespoke tuning of multiple parameters to produce reasonable results. Thus, at a practical level, it is often unclear which method should be used, how to choose parameters, and how to compare results from different methods.

The ability to assess the most appropriate derivative estimation algorithm to use based upon features of the data is of paramount importance. Currently, practitioners must often implement a number of methods, relying on disparate software packages, before selecting one that is appropriate for their application. Whereas high-quality data can leverage simple and computationally efficient algorithms (e.g. finite-differences), data that are sparse and noisy requires more sophisticated algorithms that are also more computationally expensive (e.g. total variation regularization). Regardless of application domain, scientists of various levels of mathematical expertise would benefit from a unified toolbox for differentiation techniques and parameter tuning. To address these needs, we built the open-source package PyNumDiff, with two primary goals in mind: (1) to develop a unified source for a diversity of differentiation methods using a common API, and (2) to provide an objective approach for choosing optimal parameters with a single universal hyperparameter ( $\gamma$ ) that functions similarly for all differentiation methods (Van Van Breugel et al., 2020). By filling these needs, PyNumdiff facilitates easy computations of derivatives on diverse time-series data sets.

## Summary

PyNumDiff is a Python package that implements methods for computing numerical derivatives of noisy data. In this package, we implement four commonly used families of differentiation methods whose mathematical formulations have different underlying assumptions, including both global and local methods (Ahnert & Abel, 2007). The first family of methods usually start by applying a smoothing filter to the data, followed by a finite difference calculation (Butterworth & others, 1930). The second family relies on building a local model of the

<sup>\*</sup>corresponding author

data through linear regression, and then analytically calculating the derivative based on the model (Belytschko et al., 1996; Savitzky & Golay, 1964; Schafer, 2011). The third family we consider is the Kalman filter (Aravkin et al., 2017; Crassidis & Junkins, 2004; Henderson, 2010; Kalman, 1960), with unknown noise and process characteristics. The last family is an optimization approach based on total variation regularization (TVR) method (Chartrand, 2011; Rudin et al., 1992). For more technical details, refer to (Van Van Breugel et al., 2020). Individual methods under each family are accessed through the API as `pynumdiff.family.method`.

Applying PyNumDiff usually takes three steps: (i) pick a differentiation method, (ii) obtain optimized parameters and (iii) apply the differentiation. Step (ii) can be skipped if one wants to manually assign the parameters, which is recommended when computation time is limited and the timeseries is long. Alternatively for long timeseries, optimal parameters can be chosen using a short but representative subset of the data. This optimization routine is provided as a sub-module (`pynumdiff.optimize`) with the same structure of differentiation families (i.e. `pynumdiff.optimize.family.method`). By default, the package performs the optimization using the open source CVXOPT package. Faster solutions can be achieved by using proprietary solvers such as MOSEK.

The software package includes tutorials in the form of Jupyter notebooks. These tutorials demonstrate the usage of the aforementioned features. For more detailed information, there is a more comprehensive Sphinx documentation associated with the repository.

## Acknowledgements

The work of J. Nathan Kutz was supported by the Air Force Office of Scientific Research under Grant FA9550-19-1-0011 and FA9550-19-1-0386. The work of F. van Breugel was supported by NIH grant P20GM103650, Air Force Research Lab award FA8651-20-1-0002 Airforce Office of Scientific Research FA9550-21-0122. BWB acknowledges support from the Air Force Office of Scientific Research award FA9550-19-1-0386.

## References

- Ahnert, K., & Abel, M. (2007). Numerical differentiation of experimental data: Local versus global methods. *Computer Physics Communications*, 177(10), 764–774.
- Aravkin, A., Burke, J. V., Ljung, L., Lozano, A., & Pillonetto, G. (2017). Generalized kalman smoothing: Modeling and algorithms. *Automatica*, 86, 63–86.
- Belytschko, T., Krongauz, Y., Organ, D., Fleming, M., & Krysl, P. (1996). Meshless methods: An overview and recent developments. *Computer Methods in Applied Mechanics and Engineering*, 139(1-4), 3–47.
- Butterworth, S., & others. (1930). On the theory of filter amplifiers. *Wireless Engineer*, 7(6), 536–541.
- Chartrand, R. (2011). Numerical differentiation of noisy, nonsmooth data. *International Scholarly Research Notices*, 2011.
- Crassidis, J. L., & Junkins, J. L. (2004). *Optimal estimation of dynamic systems* (Vol. 2). Chapman & Hall/CRC Boca Raton, FL.
- Henderson, G. (2010). Fundamentals of kalman filtering: A practical approach—third edition. Progress in aeronautics and astronautics series vol. 232 p. Zarchan and h. Musoff american institute of aeronautics and astronautics, 1801 alexander bell drive, suite 500, reston, VA 20191-4344, USA. 2009. Distributed by transatlantic publishers group, unit 242, 235 earls court road, london, SW5 9FE, UK.(tel: 020-7373 2515; e-mail:-richard@

- 83 tpgltd. Co. Uk). 853pp. Illustrated.£ 100.[10% discount available to RAeS members on  
84 request]. ISBN 978-1-60086-718-7. *The Aeronautical Journal*, 114(1152), 121–122.
- 85 Kalman, R. E. (1960). *A new approach to linear filtering and prediction problems*.
- 86 Rudin, L. I., Osher, S., & Fatemi, E. (1992). Nonlinear total variation based noise removal  
87 algorithms. *Physica D: Nonlinear Phenomena*, 60(1-4), 259–268.
- 88 Savitzky, A., & Golay, M. J. (1964). Smoothing and differentiation of data by simplified least  
89 squares procedures. *Analytical Chemistry*, 36(8), 1627–1639.
- 90 Schafer, R. W. (2011). What is a savitzky-golay filter?[lecture notes]. *IEEE Signal Processing*  
91 *Magazine*, 28(4), 111–117.
- 92 Van Van Breugel, F., Kutz, J. N., & Brunton, B. W. (2020). Numerical differentiation of noisy  
93 data: A unifying multi-objective optimization framework. *IEEE Access*, 8, 196865–196877.

DRAFT