NoisySignalIntegration.jl: A Julia package for uncertainty evaluation of numeric integrals

Nils O. B. Lüttschwager[1]

1 Georg-August-University Göttingen, Institute of Physical Chemistry, Tammannstraße 6, DE-37077 Göttingen

DOI: 10.21105/joss.03526

Software

- Review
- Repository
- Archive

Editor: Mehmet Hakan Satman

Reviewers:

- @myousefi2016
- @mseri

Submitted: 08 July 2021
Published: 31 August 2021

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

Summary

The evaluation of peak or band areas is a recurring task in scientific data evaluation. For example, in molecular spectroscopy, absorption line or band areas are often used to determine substance abundance. NoisySignalIntegration.jl provides functionality to evaluate such signal areas and associated uncertainties using a Monte-Carlo approach. Uncertainties may include contributions from (potentially correlated) Gaussian noise, baseline subtraction, and uncertainty in placing integration bounds. Uncertain integration bounds can be defined in several ways to constrain the integration based on the physical system under investigation (asymmetric signals, symmetric signals, signals with identical width). The package thus offers a more objective uncertainty evaluation than a statement based on experience or laborious manual analysis (Gottschalk et al., 2018).

NoisySignalIntegration.jl includes a detailed documentation that covers the typical workflow with several examples. The API uses custom datatypes and convenience functions to aid the data analysis and permits flexible customizations: Any probability distribution from Distributions.jl (Besançon et al., 2021; Lin et al., 2019) is a valid input to express uncertainty in integration bounds, thus allowing to adapt the uncertainty analysis as needed to ones state of knowledge. The core integration function can be swapped if the included trapezoidal integration is deemed unsatisfactory in terms of accuracy. The package uses MonteCarloMeasurements.jl (Bagge Carlson, 2020) to express uncertain numbers which enables immediate uncertainty propagation.

Statement of need

Several open source options for uncertainty propagation are available, e.g. the Python packages uncertainties (Lebigot) or MetroloPy (Parks, 2021) or Julia packages Measurements.jl (Giordano, 2016) and the aforementioned MonteCarloMeasurements.jl (Bagge Carlson, 2020), but uncertainty evaluation when integrating experimental x-y data is not fully addressed and requires significant effort from the user. A straightforward solution to this problem is to fit a peak function of appropriate shape and derive the uncertainty from the fit. However, the data may not be described by a peak function and/or the noise may not be normally distributed, preventing a simple least squares regression. NoisySignalIntegration.jl was developed as a solution to this problem. While the package was developed specifically for the determination of band area uncertainties in the context of molecular spectroscopy (Gawrilow & Suhm, 2021; Karir et al., 2019; Zimmermann et al., 2021), it is applicable in any research area where signals (peaks, lines, bands, etc.)[1] in x-y data need to be integrated and a thorough uncertainty analysis is desired.

[1]The name usually depends on the specific area and context.

Acknowledgements

The author thanks Charlotte Zimmermann, Maxim Gawrilow, and Robert Medel for testing and discussions during the development of NoisySignalIntegration.jl. The development has furthermore profited from the benchmarking spirit and efforts in the DFG research training group GRK 2455/389479699 to analyse experiments as rigorously as possible.

References

Bagge Carlson, F. (2020). *MonteCarloMeasurements.jl: Nonlinear propagation of arbitrary multivariate distributions by means of method overloading*. arXiv:2001.07625. https://arxiv.org/abs/2001.07625

Besançon, M., Papamarkou, T., Anthoff, D., Arslan, A., Byrne, S., Lin, D., & Pearson, J. (2021). Distributions.jl: Definition and modeling of probability distributions in the JuliaStats ecosystem. *Journal of Statistical Software*, *98*(16), 1–30. https://doi.org/10.18637/jss.v098.i16

Gawrilow, M., & Suhm, M. A. (2021). Quantifying conformational isomerism in chain molecules by linear Raman spectroscopy: The case of methyl esters. *Molecules*, *26*, 4523. https://doi.org/10.3390/molecules26154523

Giordano, M. (2016). *Uncertainty propagation with functionally correlated quantities*. arxiv:1610.08716. https://arxiv.org/abs/1610.08716

Gottschalk, H. C., Poblotzki, A., Suhm, M. A., Al-Mogren, M. M., Antony, J., Auer, A. A., Baptista, L., Benoit, D. M., Bistoni, G., Bohle, F., Dahmani, R., Firaha, D., Grimme, S., Hansen, A., Harding, M. E., Hochlaf, M., Holzer, C., Jansen, G., Klopper, W., … Mata, R. A. (2018). The furan microsolvation blind challenge for quantum chemical methods: First steps. *The Journal of Chemical Physics*, *148*(1), 014301. https://doi.org/10.1063/1.5009011

Karir, G., Lüttschwager, N. O. B., & Suhm, M. A. (2019). Phenylacetylene as a gas phase sliding balance for solvating alcohols. *Physical Chemistry Chemical Physics*, *21*, 7831–7840. https://doi.org/10.1039/C9CP00435A

Lebigot, E. O. *Uncertainties: A python package for calculations with uncertainties*. https://uncertainties-python-package.readthedocs.io

Lin, D., White, J. M., Byrne, S., Bates, D., Noack, A., Pearson, J., Arslan, A., Squire, K., Anthoff, D., Papamarkou, T., Besançon, M., Drugowitsch, J., Schauer, M., & other contributors. (2019). *JuliaStats/Distributions.jl: a Julia package for probability distributions and associated functions*. https://doi.org/10.5281/zenodo.2647458

Parks, H. V. (2021). MetroloPy. *GitHub Repository*. https://github.com/nrc-cnrc/MetroloPy/

Zimmermann, C., Lange, M., & Suhm, M. A. (2021). Halogens in acetophenones direct the hydrogen bond docking preference of phenol via stacking interactions. *Molecules*, *26*, 4883. https://doi.org/10.3390/molecules26164883