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

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., 2019; 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 (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 (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), 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.

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

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