

# PyUnfold: A Python package for iterative unfolding

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## Summary

PyUnfold is an extensible framework for the deconvolution of discrete probability distributions via the iterative unfolding method described in (D’Agostini 1995). This method falls into the general class of inverse problems, and is especially powerful when no analytic form of the inverse function is explicitly available, instead requiring an estimate (e.g. via a finite amount of simulation) of the response function. Given that measured data comprise a finite sample, PyUnfold also implements the uncertainty contributions stated in (Adye 2011).

The primary purpose of PyUnfold is to provide an unfolding toolkit for members of all scientific disciplines in an easy-to-use package. For example, unfolding methods are commonly used in the analysis pipeline of the high-energy physics (HEP) community. However, the deconvolution packages used in HEP maintain a strong dependence on the ROOT data analysis framework (ROOT 1997), which is almost exclusively used in HEP. Instead, PyUnfold is built on top of the Python scientific computing stack (i.e. NumPy, SciPy, and pandas), thus broadening its scope to a general scientific audience.

Indeed, the method itself is data-agnostic, referring to the measurement process as the smearing of a set of true causes into a set of detectable effects. For example one could define as causes the true energy of a particle and the effects the measured energy of that particle in a detector. Another example might be a set of diseases (causes) and possible clinical symptoms (effects). So long as it is possible to encode estimable resolutions and biases connecting causes to effects in a binned response matrix, one can perform a deconvolution with PyUnfold.

PyUnfold has been designed to be both easy to use for first-time users as well as flexible enough for fine-tuning an analysis. Its main strength is its simplicity, requiring a single line to run via the `iterative_unfold` method, taking as input the user provided distributions and other runtime parameters. This also facilitates examining the effects of varying optional parameters on the final unfolded distribution, allowing users to seamlessly test the robustness of results.

PyUnfold provides support for the following:

- Custom, user defined initial prior probability distributions, the default being the uniform prior. The non-informative Jeffreys’ prior (Jeffreys 1946) is accessible as a utility function.
- Unfolding stopping criteria based on test statistic calculations comparing unfolded distributions from one iteration to the next. These include Kolmogorov-Smirnov (Kolmogorov 1933) (Smirnov 1948),  $\chi^2$ , relative difference, and Bayes factor (BenZvi et al. 2011) tests.
- Tunable spline regularization as a means of ensuring that unfolded distributions do not suffer from growing fluctuations potentially arising from the finite binning of

the response matrix.

- Option to choose between Poisson or multinomial forms of the covariance matrices for both the data and response contributions to the uncertainty calculation.
- Multivariate unfolding via definitions of subsets of causes, which are regularized in their respective blocks or groups.

Further mathematical details regarding the iterative unfolding procedure, including complete derivations of the statistical and systematic uncertainty propagation can be found in the L<sup>A</sup>T<sub>E</sub>X documentation.

PyUnfold has been applied successfully for the measurement of the cosmic-ray energy spectrum by the HAWC Observatory (Alfaro, R. and others 2017) and is currently being used in an analysis by members of the IceCube Neutrino Observatory.

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