




Fitspy: A Python package for spectral decomposition

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Summary

Fitspy is a dedicated tool to fit spectra in python. Spectrum decomposition (also known as fitting) is the choice of a linear combination of peak models to best represent an experimental spectrum. Fitspy currently has implementations for Gaussian, Lorentzian, related asymmetric functions and the Pseudovoigt as peak models. User-defined models can also be added. For the fitting, the model parameters can be subject to bounds and constraints. From a practical point of view, the Fitspy GUI (see [Figure 1](#)) is designed to be as simple and intuitive to use as possible.

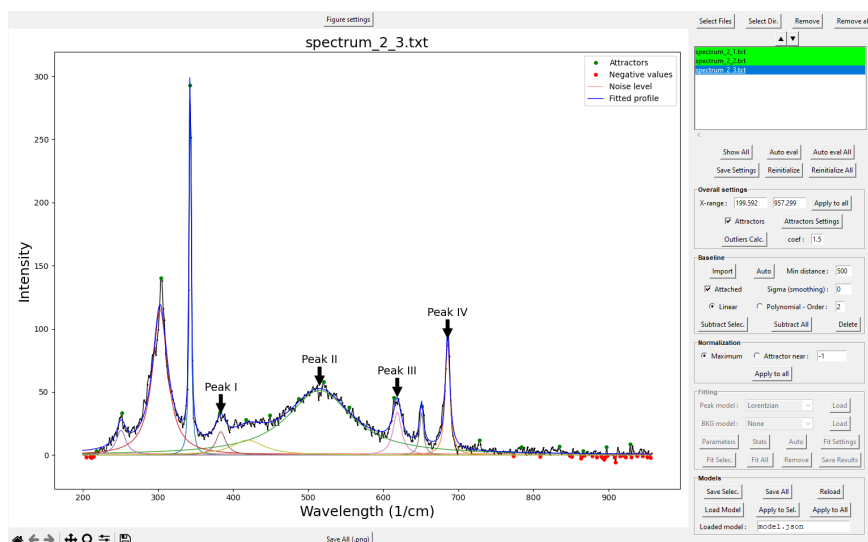


Figure 1: The Fitspy GUI featuring application options on the right-hand side, and in the central area, the current experimental spectrum displayed in black, the corresponding fit in blue, and the various modeled peaks shown in different colors.

Statement of need

The analysis of spectra in many areas of physics, from materials characterisation to astrophysics, often requires their decomposition into more or less complex models to estimate the composition of the subject being analysed. To carry out these decompositions, research communities can rely on spectral decomposition tools. While many open-source tools for spectral decomposition exist, most of them have, however, been designed for specific application domains, offering a broad range of services beyond mere spectral fitting. Consequently, these tools can prove challenging to use, especially for less experienced individuals.

In the vein of generic tools like Fityk ([Wojdyr, 2010](#)) or PRISMA ([Flores et al., 2022](#)), Fitspy

is a dedicated tool for spectral fitting — and only spectral fitting — with the following characteristics or functionalities:

- **Agnostic Nature:** Fitspy is not tied to any specific physical quantity or database. It is designed to process spectra regardless of their x-support and y-intensity without any prior knowledge.
- **Python Implementation:** Fitspy is coded in Python. As a result, for individuals with basic knowledge of the language, spectra can be easily processed by scripts.
- **User Models:** Fitspy allows the user to input their own models either in the form of literal expressions (for simple models) or through Python scripts (for more complex models).
- **2D Maps:** Fitspy has been designed to handle spectra derived from 2D acquisitions. Note that “2D” can encompass time or any other dimension. When dealing with 2D data, an interactive map in the Fitspy GUI allows the user to locate and select spectra of interest easily.
- **Multiprocessing Capabilities:** Fitspy enables spectral fit processing on multiple processors, enhancing efficiency.
- **Constrained Parameters:** Leveraging the `lmfit` library (Newville et al., 2014), Fitspy empowers the user to impose constraints on parameter ranges or establish constraints between parameters using literal expressions.
- **Simple GUI:** Fitspy has been designed to be as intuitive and simple to use as possible (subjective criterion).

To the author's knowledge, although other open-source software packages are much more advanced in certain aspects mentioned, none of them seem to encompass all the functionalities described above. Therefore, the features of Fitspy make it an ideal tool for quickly fitting a few spectra through its GUI or for fitting several thousand of spectra (or more) by Python batches, as can occur in the context of large-scale parametric studies (Meyer et al., 2023).

Fitspy workflow short description

Fitspy accepts at the time of writing two types of input data file formats:

- a first format where each spectrum is stored individually in a `.txt` file. The input data file consists of a two-column base format, with the first column containing the physical support of the spectrum (typically wavelengths) and the second to the corresponding spectrum intensity.
- the second format is associated with 2D-maps of spectra acquisitions. The related spectra are stored in a single file in which each spectrum is identified by its grid coordinates (X,Y).

Once loaded in the GUI via a files selection widget, the spectra can be processed one by one or in groups (depending on spectra selected with the cursor in the file selection widget), or as a whole dataset.

Firstly, the user can choose to reduce the physical support (wavelength axis) to a range of interest for subsequent processing. They can also activate the Attractors capability, which automatically returns the local maxima of spectra obtained with the `signal.find_peaks()` function of the `scipy` library (Gommers et al., 2023). These attractors can be used subsequently to normalise spectra or to select points associated with the baseline and peaks to be modelled (see below).

Once the range of interest and the spectra are (optionally) normalised, the user can define a **baseline** so that the spectra have a common, flat zero-intensity level. This baseline can

be defined in an automatic way or by the user, who positions characteristic points on the figure with the cursor. These points can be left at their initial positions or attached to the spectrum profile (Attached mode). In the latter case, the points can be attached either to the raw spectrum or to an averaged spectrum if the user wishes to attenuate the effects of noise. The baseline is then approximated over the entire spectrum range using either piecewise linear interpolation or an n -order polynomial approximation.

Once the baseline has been subtracted, the next step consists of defining the **peaks** of interest for the decomposition. This can be done either directly in the figure by clicking, or by an Auto mode which consists of an iterative process to automatically determine the main peak locations. Each peak is associated with a model, which can be either a predefined `Fitspy` model (Gaussian model, Lorentzian model, their asymmetric variants, or a PseudoVoigt model) or a user-defined model issued from literal expressions in a `.txt` file or from a Python script in a `.py` file. These models rely essentially on 3 main parameters: a position, an amplitude and a width (full-width half-maximum, FWHM) which is divided into *left* and *right* component for an asymmetric model.

For the fit, an additional background model can be added. Similar to peak models, background models can be defined using pre-defined models provided by `Fitspy` (Constant, Linear, Parabolic or Exponential) or by loading user-defined models from `.txt` or `.py` files.

Bounds can be imposed for each of the parameters as well as associated **constraints**. If required, these constraints can be used to link model parameters with each other, for instance in the case where a physical ratio between the amplitudes of two peaks is expected.

Finally, the parameters can be free to evolve during the fit processing or maintained fixed at their initial values.

Several fit options are also proposed, such as:

- taking into account only the positive values of the spectra.
- a (limited) choice of minimisation algorithms
- the maximum number of fit iterations
- the number of CPUs to be used during the fit processing.

At the end of the fit, the fit parameters and the statistics returned by `lmfit` are displayed in related widgets and can be exported in `.csv` and `.txt` files respectively.

All the processing steps previously described constitute a model in the sense of the `Fitspy` application that can be saved (in a `.json` file) and easily replayed as-is or applied to other spectra datasets.

In terms of visualisation, the GUI allows the user to display all of the spectra simultaneously (Show All mode) or, when a spectrum is selected, to display the corresponding fit decomposition and its residual. Figure titles and axis names can be customised and peak models labeled.

All the actions described above can be performed through Python scripts without using the GUI. In practice, when performing repeated analyses, users familiar with Python may find it helpful to use `Fitspy` as follows:

1. create a `Fitspy` model with the GUI
2. save the model
3. apply the model to several datasets using a Python script

This approach has recently been used by Meyer ([Meyer et al., 2023](#)) to process tens of thousands of PhotoLuminescence and Raman spectra acquired on wafers, taking advantage of the parallelism capabilities offered by `Fitspy` (see [Figure 2](#)).

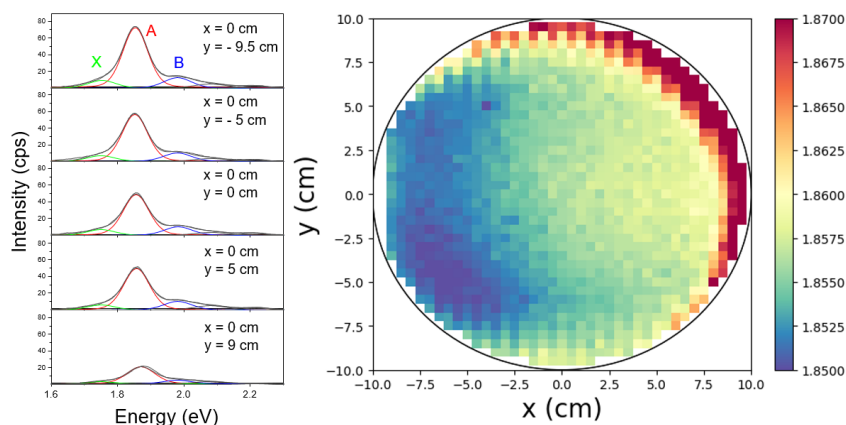


Figure 2: Example of a Fitypy application used in photoluminescence to characterise exciton intensities on a wafer (Meyer et al., 2023).

Acknowledgements

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