FittingFunctions2.0

Improved version of the fittingfunctions python module used by the Physics Institution and LTH at Lund University.

Made in python version 3.11.5

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Contents

Importing

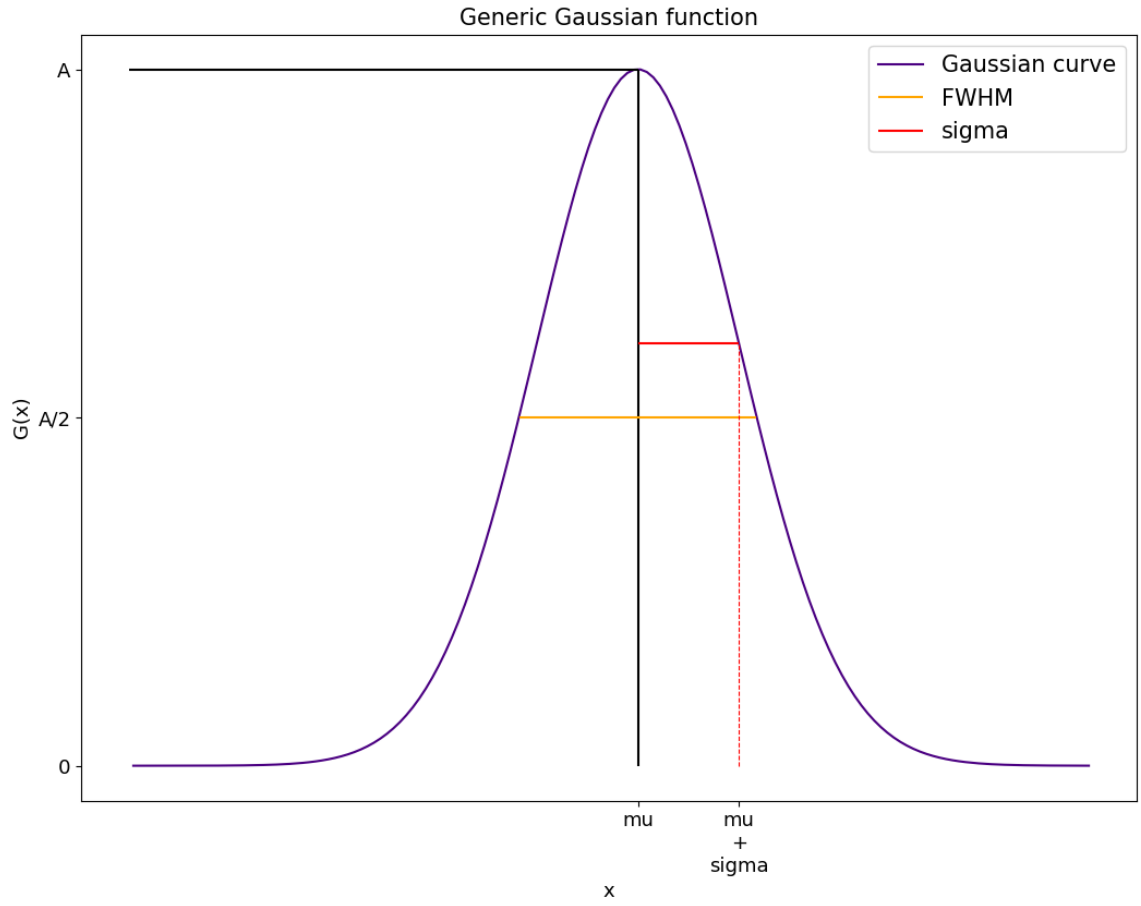
To import the module, folder FittingFunctions2 is placed in the working directory for the project and imported into the main file:

```
import FittingFunctions2 as ff
```

Gaussian Functions

For the following scripts the definition of a Gaussian function is as follows:

$$G(x) = A \cdot exp\left(-\frac{(x-mu)^2}{2\cdot(sigma)^2}\right)$$



Other useful analytical formulae are:

$$\text{Area: } area = A \cdot sigma \cdot \sqrt{2 \cdot \pi}$$

$$\text{Full-Width-Half-Maximum: FWHM } = sigma \cdot 2\sqrt{2\pi}$$

gaussian class

The gaussian class holds the return values from all functions that fit a Gaussian function and is not intended to be used independently. **Printing** a gaussian object gives rounded values. Raw values are accessed as public members or methods. Raw values for uncertainties have to be derived from the covariance matrix.

Printing

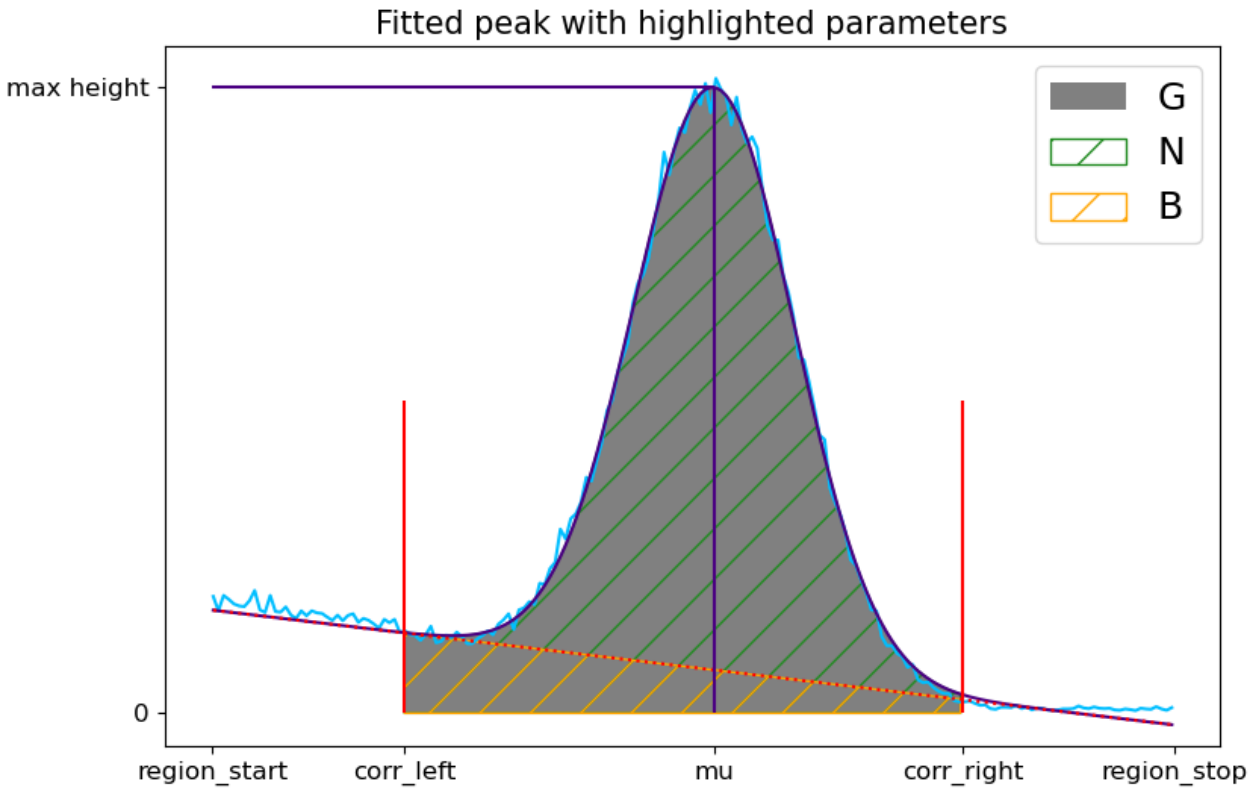
Example of a gaussian fitted to a Cs-137 peak in a gamma ray spectrum.

```
[Python3]: print(BGO["662kev"])
========================= Gaussian Peak =========================
Estimated parameters: A = 1740.5264, mu = 661.8352, sigma = 40.6196
Uncertainties: σ(A) = 7.7571, σ(mu) = 0.2089, σ(sigma) = 0.2096
Additional info: Max height = 1915.892, G = 79320, N = 65096, B = 14224

Covariance matrix:
 [[ 6.01726192e+01  1.87206691e-03 -9.40087680e-01]
```

```
    [ 1.87206691e-03  4.36592014e-02 -9.98241359e-05]
    [-9.40087680e-01 -9.98241359e-05  4.39143608e-02]]
```

Generic peak



Public members

Member	Description
*gaussian.***A** : *float*	The amplitude of the fitted function. OBS! This does not account for the scatter correction and will sometimes not match the peak height in a spectrum, see *gaussian.max_height()*.
*gaussian.***mu** : *float*	The central value of the fitted gaussian curve.
*gaussian.***sigma** : *float*	The fitted value of sigma.
*gussian.***cov_matrix** *3x3-array*	The covariance matrix from the fit corresponding to *A, mu* and *sigma*.
*gussian.***G** : *float*	The gross area of the region enclosed by the scatter correction boundaries, i.e. the sum of all y-values in the selected region.
*gussian.***B** : *float*	The scatter background calculated as the sum of the linear scatter correction function across the region enclosed by the scatter correction boundaries.

Member	Description
gussian.**N** : *float*	The net area of the peak, i.e. *gussian*.**G** - *gussian*.**B**.

Public Methods

Method	Description
gussian.**area()** : *-> float*	The analytically calculated area of the gaussian. OBS! This may deviate from *gaussian.G* as the bin size in the x-data is not accounted for by this function.
gussian.**FWHM(uncertanty = False** *: bool* **)** : *-> float/tuple*	Return the full-width-half-max value of the peak. Setting *uncertanty* till *True* return a tuple with the FWHM as the first element the uncertainty in FWHM as the second.
gussian.**max_height()** : *-> float*	Returns the real height of the gaussian at the point *mu*. Calculated as corr_f(mu) + A.
gussian.**plot(xlabel = None** *: str* **, ylabel = None** *: str* **)** : *-> None*	Plots the gaussian over the selected region.
gussian.**value(x** *: float* **)** : *-> float*	Returns the value of the gaussian at the point *x*.

Fitting Functions

fit_gaussian

```
fit_gaussian(X, Y, region_start, region_stop,
             corr_left=None, corr_right=None,
             mu_guess=None, A_guess=None, sigma_guess=None,
             scatter_corr="auto", scatter_corr_points=3,
             corr_thresh=0.05)
```

Attempts to fit a gaussian function to a data set using the *curve_fit* routine from scipy.optimize.

Parameter	Description
X : *array_like*	An array corresponding to the x-axis of the data set.
Y : *array_like*	An array corresponding to the y-axis of the data set.
region_start : *float*	The lower bound of the region on which the gaussian will be fitted.
region_stop : *float*	The upper bound of the region on which the gaussian will be fitted.
corr_left : *float, optional*	Left point at which scatter correction will be made. This only affects the scatter correction, the fit will always be made over the entire region.

Parameter	Description
corr_right : *float, optional*	Right point at which scatter correction will be made. This only affects the scatter correction, the fit will always be made over the entire region.
mu_guess : *float, optional*	Manual guess for *mu*.
A_guess : *float, optional*	Manual guess for *A*.
sigma_guess : *float, optional*	Manual guess for *sigma*.
scatter_corr : *str/bool, optional*	Sets method of scatter correction. `'auto'` attempts automatic scatter correction, if this fails *region_start* and *region_stop* will be set as correction boundaries. Manually setting boundaries will overrule the automatically set boundaries. `True` makes scatter correction without automatically set limits. Limits are manually set by *corr_left* and *corr_right*, if one or both of these are not set *region_start* and *region_stop* will be set as correction points. `False` no scatter correction is made.
scatter_corr_points : *int, optional*	The number of points over which the bounds of the scatter correction is averaged. The default 3 means the point is chosen as the average of the first 3 inside the gaussian region.
corr_thresh : *float, optional*	Sets the gradient threshold for determining the edges of the peak when `sactter_corr='auto'`.

Returns	Description
Peak : *gaussian*	An object containing the data from the fit. See the section on the *gaussian* class.

`fit_double_gaussian`

Attempts to fit a sum of two gaussian functions to a data set using the *curve_fit* routine from scipy.optimize.

```
fit_double_gaussian(X, Y, region_start, region_stop, split_point,
                    corr_left=None, corr_right=None,
                    plotting = False,
                    mu1_guess=None, mu2_guess=None,
                    A1_guess=None, A2_guess=None,
                    sigma1_guess=None, sigma2_guess=None,
                    scatter_corr=True, scatter_corr_points=3)
```

Parameter	Description
X : *array_like*	An array corresponding to the x-axis of the data set.
Y : *array_like*	An array corresponding to the y-axis of the data set.

Parameter	Description
split_point : *float*	A point in between the two peaks that split the region for the purpose of automatically assigning guesses.
region_start : *float*	The lower bound of the region on which the gaussian will be fitted.
region_stop : *float*	The upper bound of the region on which the gaussian will be fitted.
corr_left : *float, optional*	Left point at which scatter correction will be made. This only affects the scatter correction, the fit will always be made over the entire region.
corr_right : *float, optional*	Right point at which scatter correction will be made. This only affects the scatter correction, the fit will always be made over the entire region.
mu1_guess / mu2_guess : *float, optional*	Manual guess for *mu*. The first peak is lower on the x-axis than the second peak, *mu1* < *mu2*.
A1_guess / A2_guess : *float, optional*	Manual guess for *A*. The first peak is lower on the x-axis than the second peak.
sigma1_guess / sigma2_guess : *float, optional*	Manual guess for *sigma*. The first peak is lower on the x-axis than the second peak.
scatter_corr : *bool, optional*	Sets if a scatter correction is made.
scatter_corr_points : *int, optional*	The number of points over which the bounds of the scatter correction is averaged. The default 3 means the point is chosen as the average of the first 3 inside the gaussian region.

Returns	Description
(peak_1, peak_2) : *tuple*	A tuple containing two *gaussian* objects corresponding to the two peaks, in order of ascending *mu* values. See the section on the *gaussian* class.

Spectrum Calibration

Calibrates a spectrum by marking peaks and providing energies corresponding to the marked peaks.

calibrate

```
calibrate(Y, peak_regions, energies, plot=False, gauss=True)
```

Parameter	Description
Y : *array_like*	The dataset corresponding to the y-axis of the spectrum.

Parameter	Description
peak_regions : *array_like*	An iterator containing start and stop values for the peak regions to be used in the calibration. A *gaussian* object can be given instead of a start and stop region. Example: `[[150, 300], (500, 600), gaussian_peak]`.
energies : *array_like*	Iterator with the energies of the peaks at the corresponding index in *peak_regions*.
plot : *bool, optional*	Plots the calibrated spectrum and highlight the points used for calibration.
gauss : *bool, optional*	If `True` a gaussian will be fitted to each selected region using the *fit_gaussian* function and the *mu* value is used as the calibration point. If `False` the maximum point in the region is used as the calibration point.

Returns	Description
calib_x : *numpy.array*	The calibrated x-axis corresponding to the given y-axis.
(k, m) : *tuple*	The calibration coefficients.

Miscellaneous

Miscellaneous functions included in the package that might be of some use.

`slice_spect`

Slices an array containing strictly increasing values, like a calibrated x-axis, based on the values in the array. More arrays of the same shape as the first array can be given and will also be sliced into the same shape as the first array.

```
slice_spect(spect, *args, low=None, high=None)
```

Parameter	Description
spect : *array_like*	An array containing a calibrated x-axis.
*args : *array_like, optional*	Additional arrays of the same shape as *spect* that will be sliced into the same shape as the returned version of *spect*
low : *float, optional*	The low cut off point for the spectrum. Both *low* and *high* can not be omitted.
high : *float, optional*	The high cut off point for the spectrum. Both *low* and *high* can not be omitted.

Returns	Description
spectra : *numpy_array / list*	If no **args* are provided only the sliced version of *spect* is returned. If **args* are provided a list is returned containing the sliced spectra in the order they are given, first being the sliced *spect*.

is_iter

```
is_iter(obj)
```

Checks if an object is iterable.

Parameter	Description
obj : *any*	Any type of object to be check if it is iterable.

Returns	Description
bool	*True* if *obj* is iterable, else *False*