Spectra Documentation

Release 0.5

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June 15, 2014

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CHAPTER ONE

SPECTRA CLASS

class `spectra.Spectra`(*filename*)

Stores spectra data in Spec (peak-o-mat) format

Methods

`build_model`(*peak_type='LO'*, *max_width=None*)

Builds a peak-o-mat model of peaks in listed by index in *peak_pos*

Parameters **peak_type** : string

Peaks can be of the following types: (to setup custom peaks and more, see peak-o-mat docs)

'LO' : symmetric lorentzian
'GA' : symmetric gaussain
'VO' : voigt profile
'PVO' : psuedo-voigt profile
'FAN' : fano lineshape

Peaks can veof default type lorentzian (LO). Uses some basic algorithms :

to determine initial parameters for amplitude and fwhm (limit on fwhm :

to avoid fitting background as peaks. :

`filter_high_freq`(*data*)

Filter high frequency data using fft

Parameters **data** : np.array

Data to filter

Returns **data** : np.array

Data with high frequcny components removed

`find_background`(*sub_range=None*, *poly_deg=3*, *smoothing=5*)

Attempts to find the background of the spectra, and updates the *bg* array

`find_fwhm`(*position*)

Find the fwhm of a point using a very simplisitic algorigthm. Could return very large width.

find_peaks (*lower=None*, *upper=None*, *threshold=5*, *limit=20*)
Find peaks in actve data set using continous wavelet transformation from *scipy.signal*

fit_data ()
Attempt to fit data using peak-o-mat Fit function with the generated model. Updates model with fit parameters.

guess_peak_width (*max_width=50*)
Find an initial guess for the peak with of the data imported, use in peak finding and model buildings and other major functions, probably should call in the constructor

Parameters **max_width** : int

Max width of peaks to search for

Notes

Locates the max value in the data Finds the peak width associated with this data

output_results ()
Output fit paramters as csv values with errors

remove_spikes (*strength=0.5*)
Attempts to remove spikes in active set using a simple test of the pixels around it. Fractional value of strength needed.

subtract_background ()
Subtract background from active spectra

CHAPTER

TWO

SAVITZKY GOLAY

savitzky_golay.**savitzky_golay**(*y*, *window_size*, *order*, *deriv=0*, *rate=1*)

Smooth (and optionally differentiate) data with a Savitzky-Golay filter. The Savitzky-Golay filter removes high frequency noise from data. It has the advantage of preserving the original shape and features of the signal better than other types of filtering approaches, such as moving averages techniques.

Parameters **y** : array_like, shape (N,)

the values of the time history of the signal.

window_size : int

the length of the window. Must be an odd integer number.

order : int

the order of the polynomial used in the filtering. Must be less then *window_size* - 1.

deriv: int :

the order of the derivative to compute (default = 0 means only smoothing)

Returns **ys** : ndarray, shape (N)

the smoothed signal (or it's n-th derivative).

Notes

The Savitzky-Golay is a type of low-pass filter, particularly suited for smoothing noisy data. The main idea behind this approach is to make for each point a least-square fit with a polynomial of high order over a odd-sized window centered at the point.

References

[R1], [R2]

Examples

```
t = np.linspace(-4, 4, 500)
y = np.exp( -t**2 ) + np.random.normal(0, 0.05, t.shape)
ysg = savitzky_golay(y, window_size=31, order=4)
import matplotlib.pyplot as plt
plt.plot(t, y, label='Noisy signal')
plt.plot(t, np.exp(-t**2), 'k', lw=1.5, label='Original signal')
```

```
plt.plot(t, ysg, 'r', label='Filtered signal')
plt.legend()
plt.show()
```

CHAPTER

THREE

DRIVER FUNCTION

Example of how to use the Spectra

3.1 Import a file

3.2 Find Peaks

Me

CHAPTER FOUR

INDICES AND TABLES

- *genindex*
- *search*

[R1] A. Savitzky, M. J. E. Golay, Smoothing and Differentiation of Data by Simplified Least Squares Procedures. Analytical Chemistry, 1964, 36 (8), pp 1627-1639.

[R2] Numerical Recipes 3rd Edition: The Art of Scientific Computing W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery Cambridge University Press ISBN-13: 9780521880688