

Mat2Dcorr - perform 2D correlation (2D-COS) analysis with Matlab

The latest version of the Mat2Dcorr toolbox is available from <http://www.peter-lasch.de/2dcorr/>

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A.) Requirements

Files

- 1.) mat2dcorr.m
- 2.) updcorrplt.m
- 3.) linescandata.mat
- 4.) readme.txt
- 5.) Mat2Dcorr.pdf (this file)

Software

Requires Matlab R2014a or newer

B.) Installation

- 1.) Copy files 1)-5) into one single directory
- 2.) Add this directory to Matlab's search path

For this start Matlab and type

```
>> addpath('Mat2DcorrPath')
```

at the Matlab command prompt, where *Mat2DcorrPath* denotes the full path

Example of *Mat2DcorrPath*: 'C:\Users\Tim\Documents\Matlab\Mat2D'

- 3.) To start mat2Dcorr type

```
>> mat2dcorr
```

at the Matlab prompt

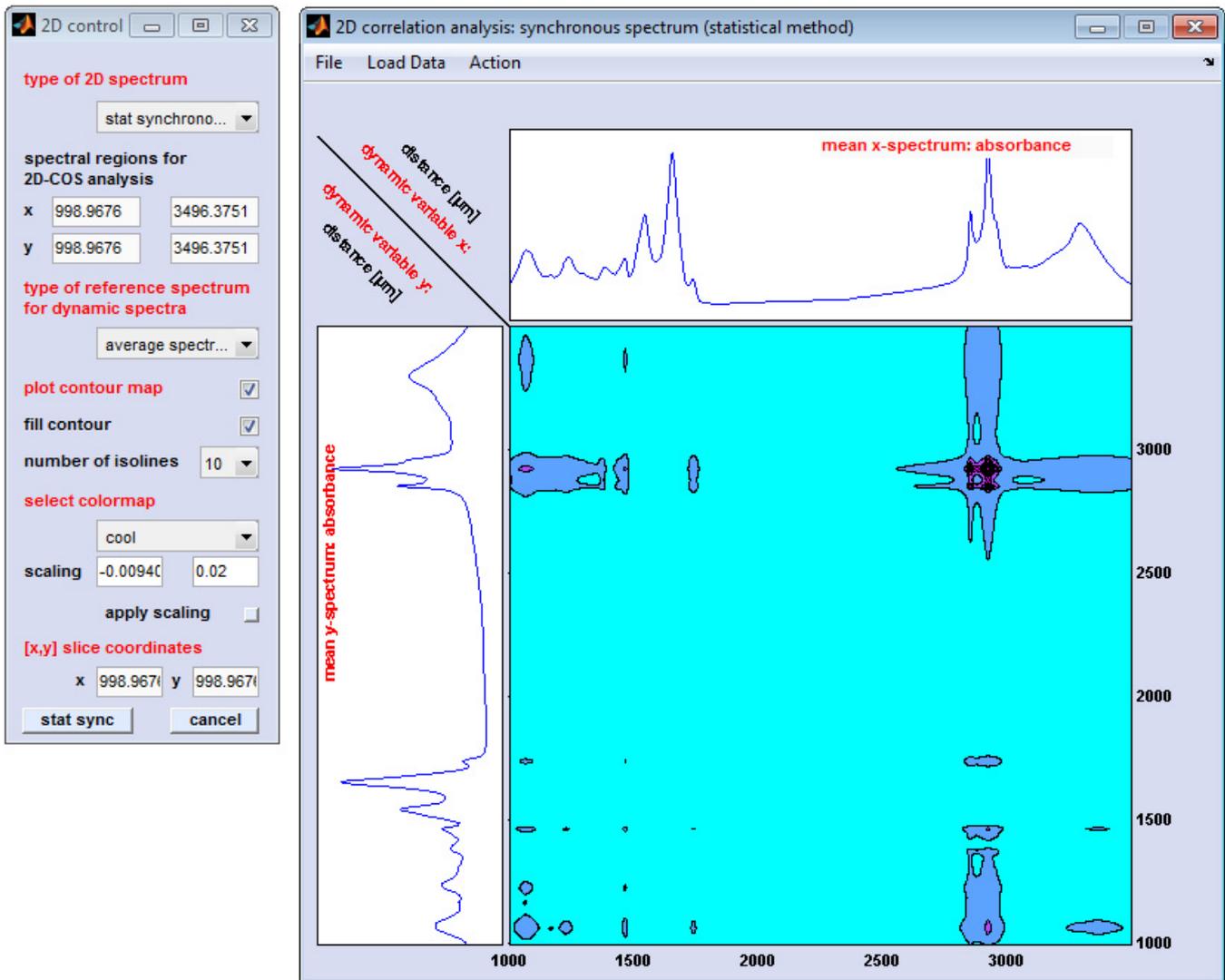
This will open two different windows

a.) A window entitled '2D correlation analysis ... ' which shows the 2D correlation spectrum and mean spectra obtained from the x- and y-spectra data

b.) The 2D-COS control window (see screenshots below)

C.) Loading Data

- 1.) Select 'Load Data' → 'Matlab imaging format' → 'x-data' to load x-data in the Matlab imaging data format. Select 'Load Data' → 'Matlab imaging format' → 'y-data' to load the respective y-data in the Matlab imaging data format. Matlab imaging data files may contain up to four different types of hyperspectral imaging data cubes: original (unprocessed data), pre-processed, derivative and so-called deconvolution data cubes (the latter 3 types of data must be derived from the original spectral data). For a detailed description of the Matlab imaging data format see <http://www.cytospec.com/file.php#FileSaveMatlab>
- 2.) Select 'Load Data' → 'Matlab trace format' → 'x-data' to load x-data in the Matlab trace data format. Select 'Load Data' → 'Matlab trace format' → 'y-data' to load the respective y-data in the Matlab trace data format.



Mat2Dcorr: screenshot of the 2D control window (left) and the window '2D correlation analysis ... ' (right)

Format of the example file 'linescandata.mat' (Matlab trace format):

Matlab trace format files contain spectra series in a 2D data format where the first dimension is the spectral dimension and the second dimension represents the perturbing variable, i.e. time, pressure, temperature, spatial dimension, etc.

Matlab trace files contain a structure array with the following fields:

- spc** - this field contains the spectral data, a 2D array of double precision floating point values (float32). Columns indicate individual spectra of absorbance, intensity, transmittance, etc. values. The column length indicates the number of data points per spectrum. The number of columns is equal to the number of spectra of the spectra series.
- wav** - A vector of float32 values, the 'wavenumber' vector, or more general the vector of y-values (frequencies, wavenumbers, Raman shifts or alternative variables). The length of 'wav' must equal the number of data points per spectrum, i.e. $\text{size}(\text{wav},1) == \text{size}(\text{spec},1)$. Equidistance of the 'wav' vector is not a requirement.
- tos** - A character vector of variable length which indicates the type of spectra. Examples: 'Transmission', 'Fluorescence', 'Raman', etc.
- war** - A vector of float32 values, which denote the perturbing variable of the experiment: temperature, time, voltage. The length of 'war' must be equal to $\text{size}(\text{spc},2)$

vst - A character vector of variable length indicating the type of the perturbing variable. Examples of vst: 'Temperature', 'Time', 'Voltage', or 'Spatial variable'

If the data were loaded successfully and the number of spectra in the x- and y-spectra files are identical, the button 'stat sync' (initially grayed out) becomes available, so 2D-COS analysis can be started.

Choose first the type of 2D-COS analysis from the popupmenu labeled as 'type of 2D spectrum'. Valid options are:

- Pearson scaling the synchronous 2D spectrum with Pearson, or unit variance scaling. Pearson scaling is also used in statistical total correlation spectroscopy [STOCSY] and statistical heterospectroscopy [SHY])
- Pareto scale 0.75 the synchronous 2D spectrum with Pareto scaling. The parameter α equals 0.75
- Pareto scale 0.50 the synchronous 2D spectrum with Pareto scaling. The parameter α equals 0.50 (Pareto scaling in the strict sense)
- Pareto scale 0.25 the synchronous 2D spectrum with Pareto scaling. The parameter α equals 0.25
- stat synchronous the classical synchronous 2D (covariance) spectrum
- stat asynchronous the classical asynchronous 2D spectrum
- disrelation allows to calculate the absolute of the 2D disrelation spectrum
- fft synchronous alternative implementation to obtain the synchronous 2D correlation spectrum by means of the fast Fourier-transformation approach
- fft asynchronous alternative implementation to obtain the asynchronous 2D correlation spectrum by means of the fast Fourier-transformation approach

A more detailed description of the Matlab toolbox Mat2Dcorr will follow soon

To be continued.