

PyLDA

Load File
Quit

A

Time and Wavelength Bounds

Time Min

Time Max

WL Min

WL Max

Update Bounds

IRF and Chirp Parameters

FWHM

μ

λ

Order

Fix Values

Fit IRF

C

LDA Options

Regularization Method Regularization Matrix

☒ Tikhonov ☒ Identity

☐ LASSO ☐ 1D

☐ Elastic Net ☐ 2D

☐ Fused

B

SVD and GA Options

Alpha

wLSVs

Initial Guess

Bounds

D

Lifetime Settings

Min Tau

Max Tau

Num Taus

☒ Log Scale ☐ Linear Scale

E

Alpha Settings

Alpha Min

Alpha Max

Num Alphas

☒ Simultaneous ☐ Independently

Run LDA

F

Low Rank Data Approximation

Truncate

E

TSVD

K

Tau Min

Tau Max

Num Taus

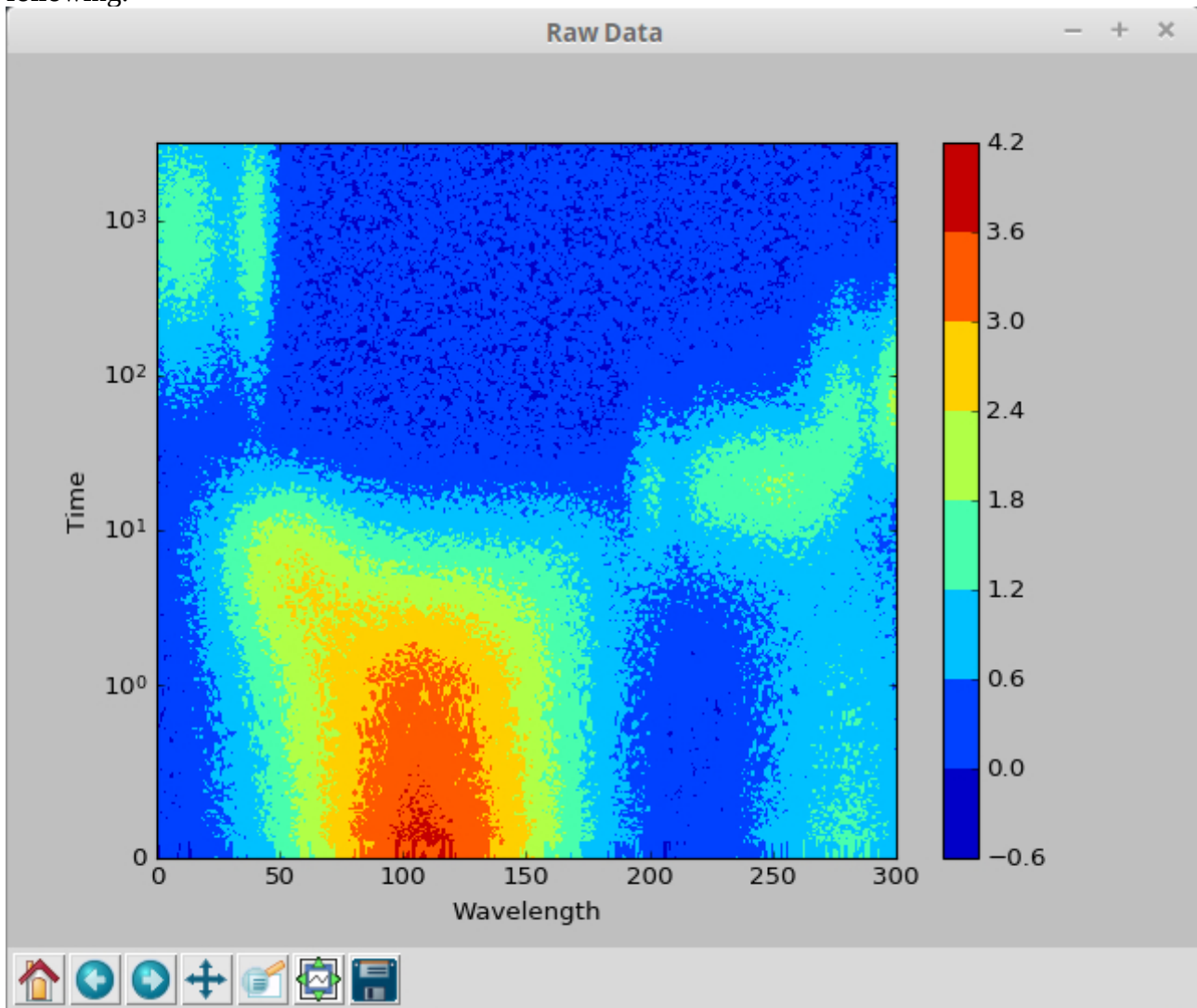
Run TSVD LDA

A

1. Data should be in absorbance (not transmission) format. The file should be a CSV with the following formatting:

,	Wavelength λ_1 ,	Wavelength λ_2 ,
Time t_1 ,	$\Delta(t_1, \lambda_1)$,	$\Delta(t_1, \lambda_2)$,
Time t_2 ,	$\Delta(t_2, \lambda_1)$,	$\Delta(t_2, \lambda_2)$,

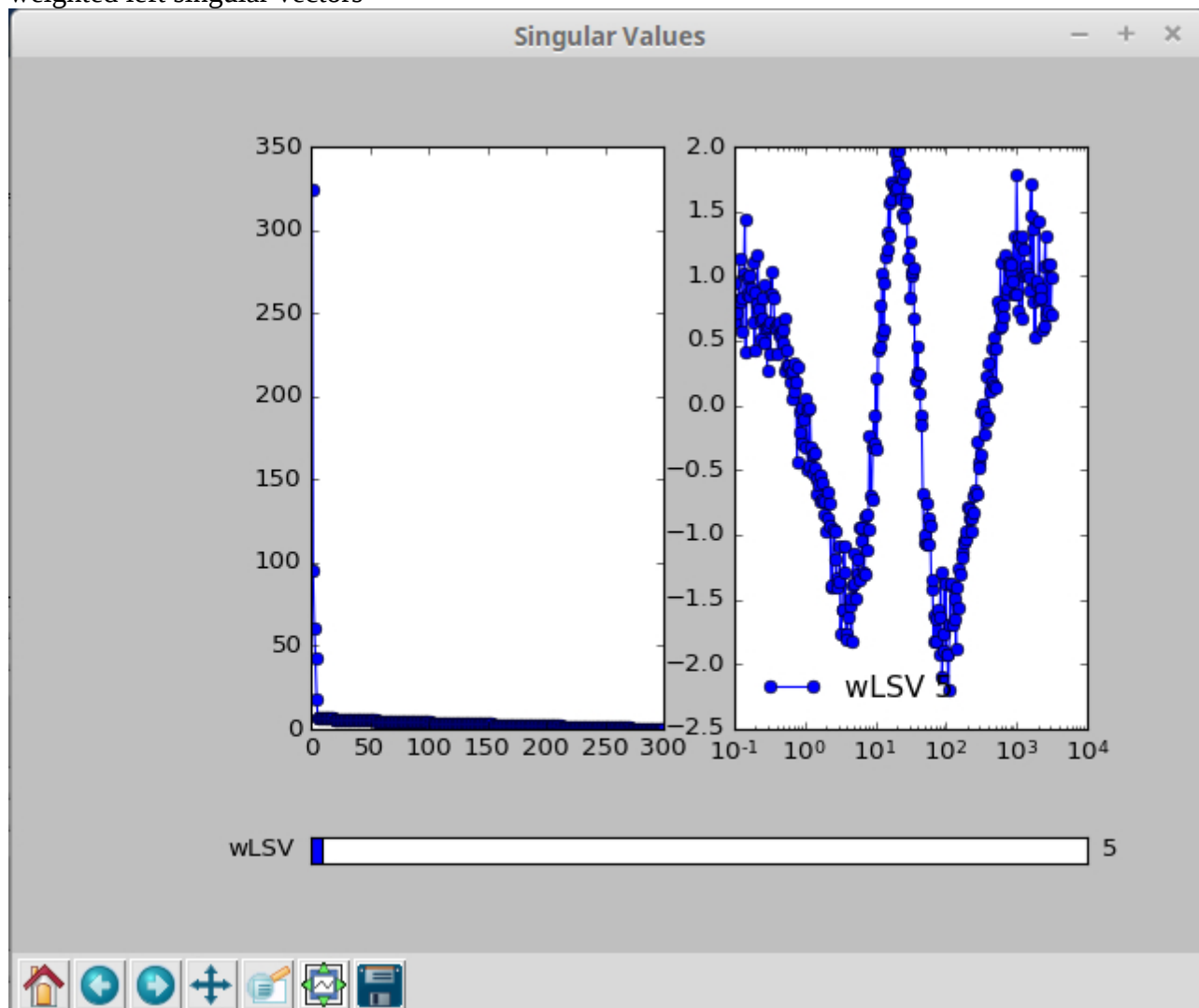
2. When the data is loaded, it will be displayed on a symbolic lin-log plot. This means that the a pseudo log scale will be used for negative time points. In addition, the plot will be linear between -1 and 1. Loading the file `synthdata_noise10.csv` from the Data subdirectory should display the following.



3. The Time min/max and Wl min/max are **indices** for the range of data to be used for fitting. By default, the minimum time point is set to the index of time zero. The wavelengths are set to the full range by default. **Note:** python indexing begins at 0, -1 indicates the last item.

B

1. Once data has been loaded, the SVD button will allow you to explore the singular values and weighted left singular vectors



2. After examining the singular values and their corresponding left singular vectors, the GA button will run a global analysis based on the input parameters.

Alpha	0
wLSVs	5
Initial Guess	1 5 10 200 2000
Bounds	,(0 10000),(0 10000)

Alpha: will allow Tikhonov regularization if set to a value other than 0. By default it is 0, corresponding to an ordinary least-squares

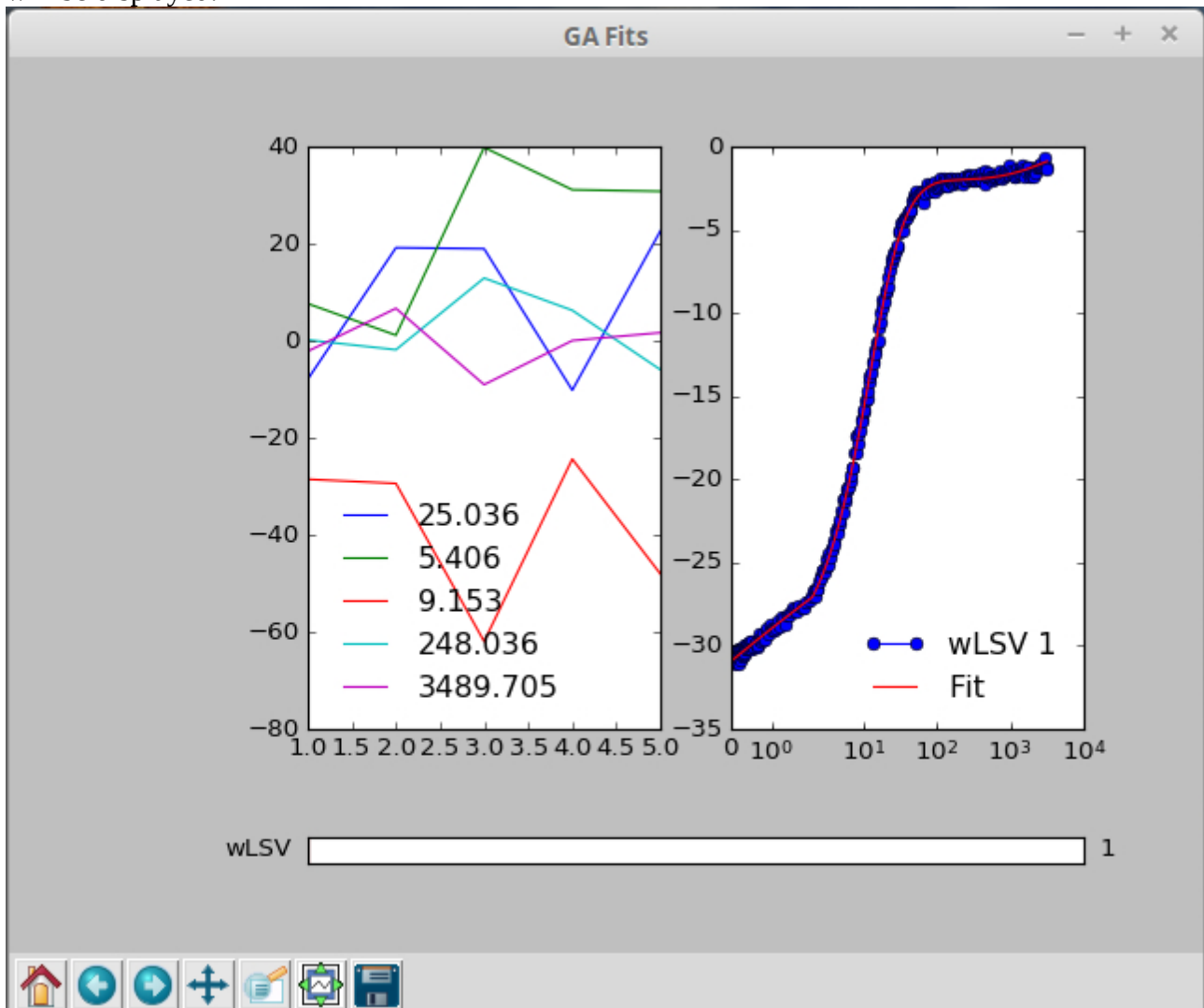
wLSVs: the number of wLSVs to include in the fit. A single number, e.g. 5, will include the first 5 vectors. Alternatively, a list can be entered to select specific vectors, with a space between the

number of each vector, e.g.: 1 2 4 5

Initial Guess: Will be a guess for each lifetime, separated by a space. The number of guesses must match the number of wLSVs used in the fit.

Bounds: Are fitting bounds for the non-linear solver. There must be a matching number of sets of bounds to number of guesses. The bounds are entered in the following format: (lower_bound upper_bound),(lower_bound2 upper_bound2),... with spaces separating the lower and upper bound for a single lifetime within the parantheses, and only a **comma** separating sets of bounds.

3. Using those values as initial parameters for the synthdata_noise10, the following results screen will be displayed:



The slider on the bottom allows you to click through each wLSV and fit. You can rerun the fitting procedure if you are unhappy with the agreement of the fit with the vectors. The left panel contains the Decay Associated Spectra (i.e. the pre-exponential functions) for the corresponding lifetimes.

C

1. These allow you to choose the type of matrix regularization and which sort of penalty matrix to use.

LDA Options

Regularization Method	Regularization Matrix
<input checked="" type="radio"/> Tikhonov	<input checked="" type="radio"/> Identity
<input type="radio"/> LASSO	<input type="radio"/> 1D
<input type="radio"/> Elastic Net	<input type="radio"/> 2D
	<input type="radio"/> Fused

The matrices are as follows:

- Identity is simply an identity matrix

- 1D is a first derivative approximation
$$\frac{1}{2} \begin{bmatrix} 1 & -1 & 0 & \dots \\ 0 & 1 & -1 & 0 & \dots \\ 0 & 0 & 1 & -1 & \dots \end{bmatrix}$$

- 2D is a second derivative approximation:

$$\frac{1}{4} \begin{bmatrix} -2 & 1 & 0 & \dots \\ 1 & -2 & 1 & 0 & \dots \\ 0 & 1 & -2 & 1 & \dots \end{bmatrix}$$

- Fused is a combination of the identity and first derivative matrices:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ \vdots & & & & \vdots \\ 1 & -1 & 0 & & \dots \\ 0 & 1 & -1 & 0 & \dots \\ 0 & 0 & 1 & -1 & \dots \end{bmatrix}$$

D

1. These settings determine the number and scale of your lifetimes, as well as the alpha selection parameters. Note that for elastic net, the rho values are simply distributed on a scale from 0 to 1 in tenths, in addition to any alpha values you select.

Lifetime Settings	
Min Tau	<input type="text" value="-1"/>
Max Tau	<input type="text" value="4"/>
Num Taus	<input type="text" value="100"/>
<input checked="" type="radio"/> Log Scale <input type="radio"/> Linear Scale	

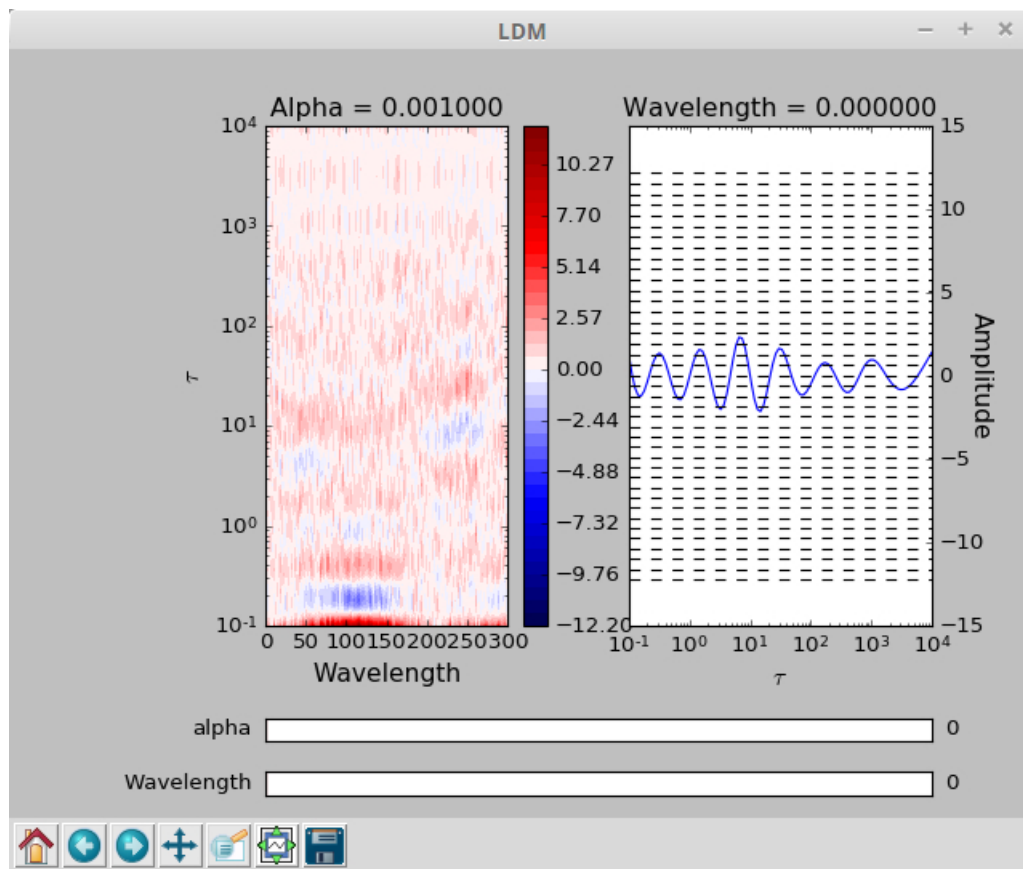
Alpha Settings	
Alpha Min	<input type="text" value="0.001"/>
Alpha Max	<input type="text" value="1.5"/>
Num Alphas	<input type="text" value="1000"/>
<input checked="" type="radio"/> Simultaneous <input type="radio"/> Independently	

The lifetimes can be distributed along a linear or log scale. Note that here they are distributed along a log scale, and thus between 10^{-1} and 10^4 .

The alphas are distributed along a linear scale. The selection of simultaneous or independently determines whether statistics are generated for all wavelengths together (simultaneous) or each independently.

2. Run LDA will produce a LDM like the following:

There will be horizontal dashed lines on the LDM corresponding to the lifetimes calculated from Global Analysis if it was run before the LDA procedure.



The alpha slider will allow you to slide through the LDMs produced at each alpha value. The right plot shows a single vertical slice through the LDM, at a particular wavelength. The wavelength slider allows you to look through the results at various wavelengths. The dashed lines represent the contour levels.

E

1. These settings are similar to those above, except for running a truncated SVD regularization instead of a matrix regularization method.

TSVD	
K	5
Tau Min	-1
Tau Max	4
Num Taus	100

Run TSVD LDA

K represents the singular value of truncation.

F

1. Pressing truncate will provide a low-rank approximation of the data matrix, with the point of truncation being the value entered in wLSVs in section B.