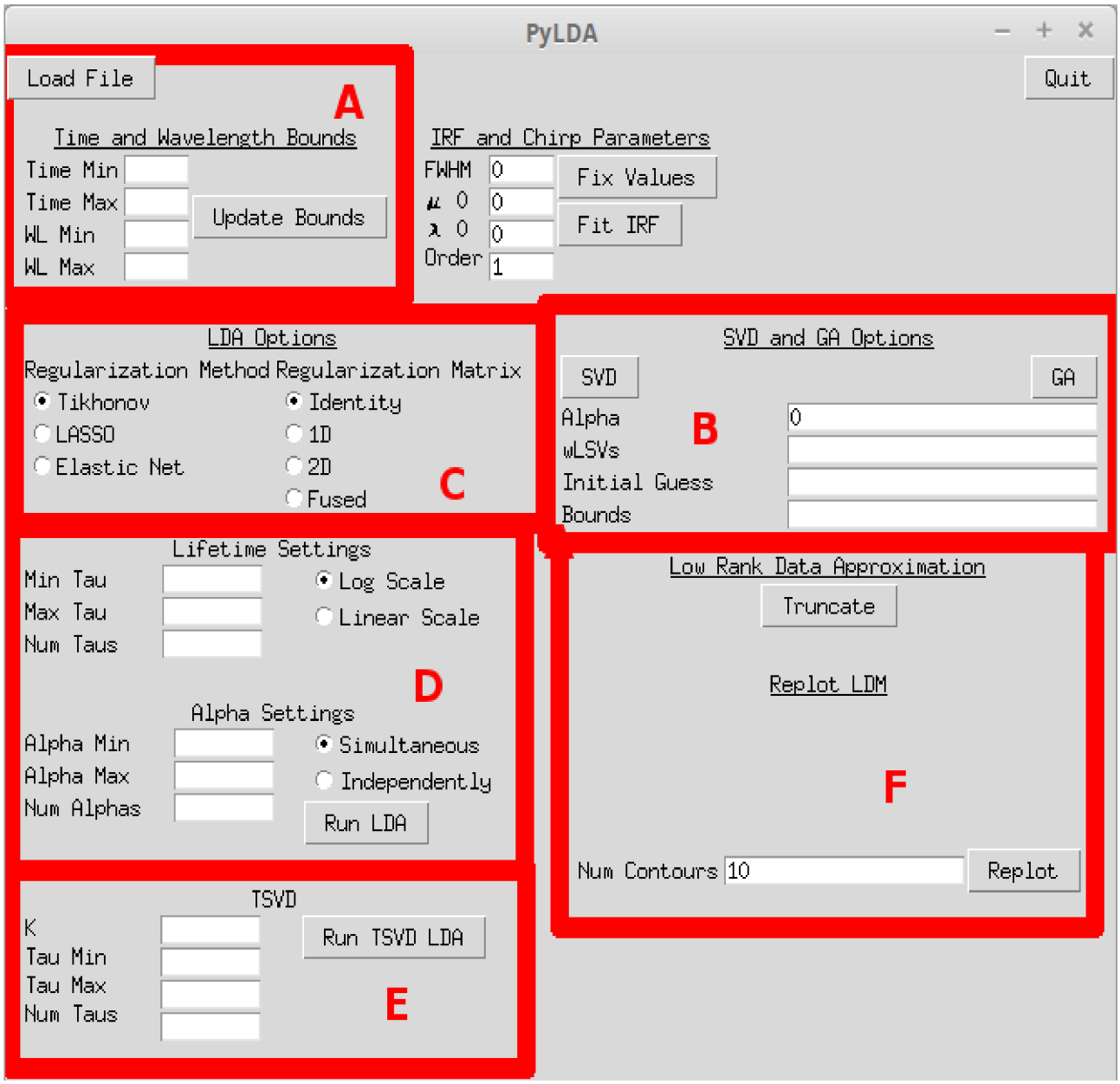
This manual will be written using the heterogenous decay data file hettaus_noise10.csv, located in the Data subdirectory. The GUI is started by running the command *python pylda.py* from the pylda directory.

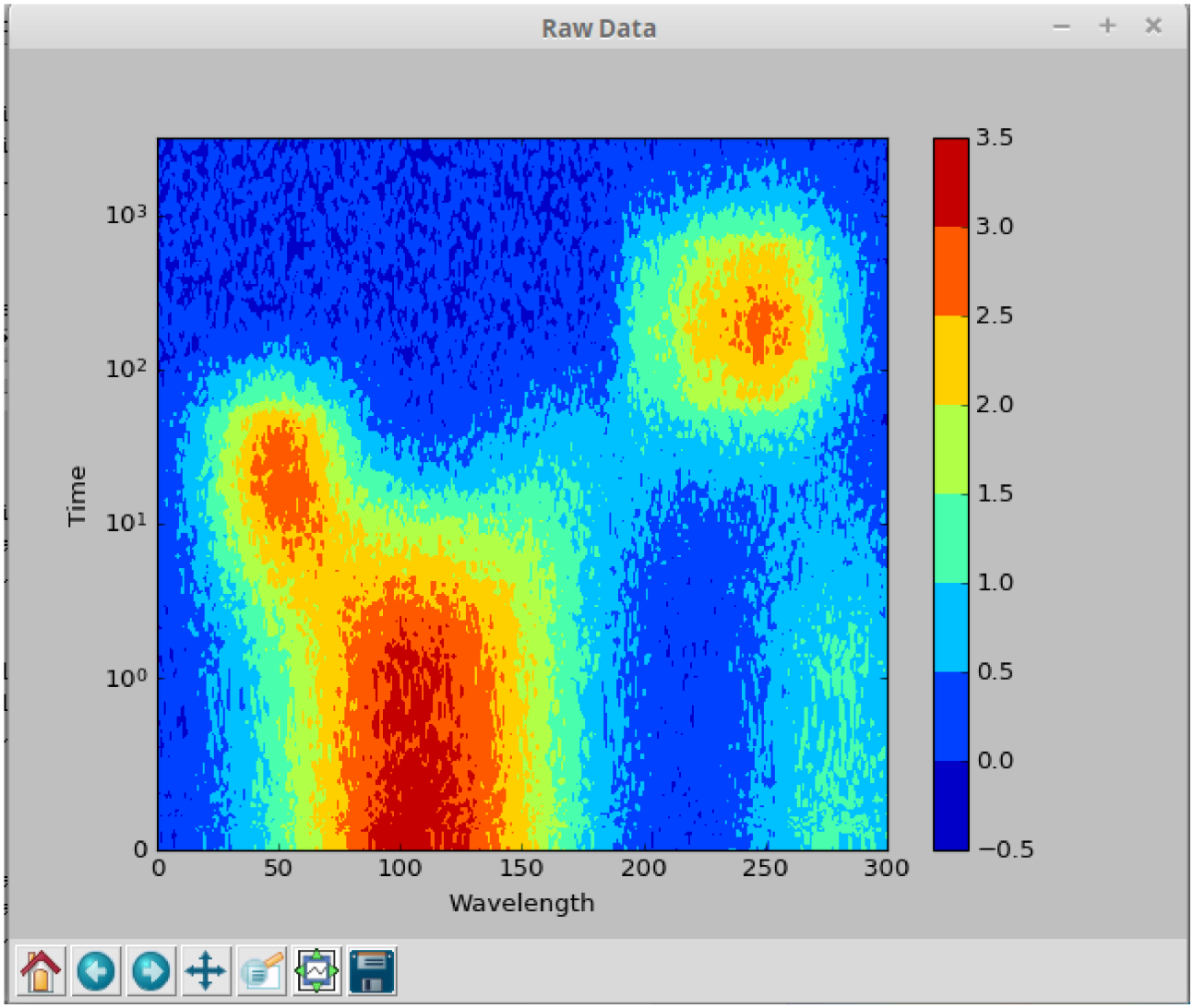


A

1. Data should be in absorbance 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 ,	**$\Delta(t_2,\lambda_1)$,**	**$\Delta(t_2,\lambda_2)$,**

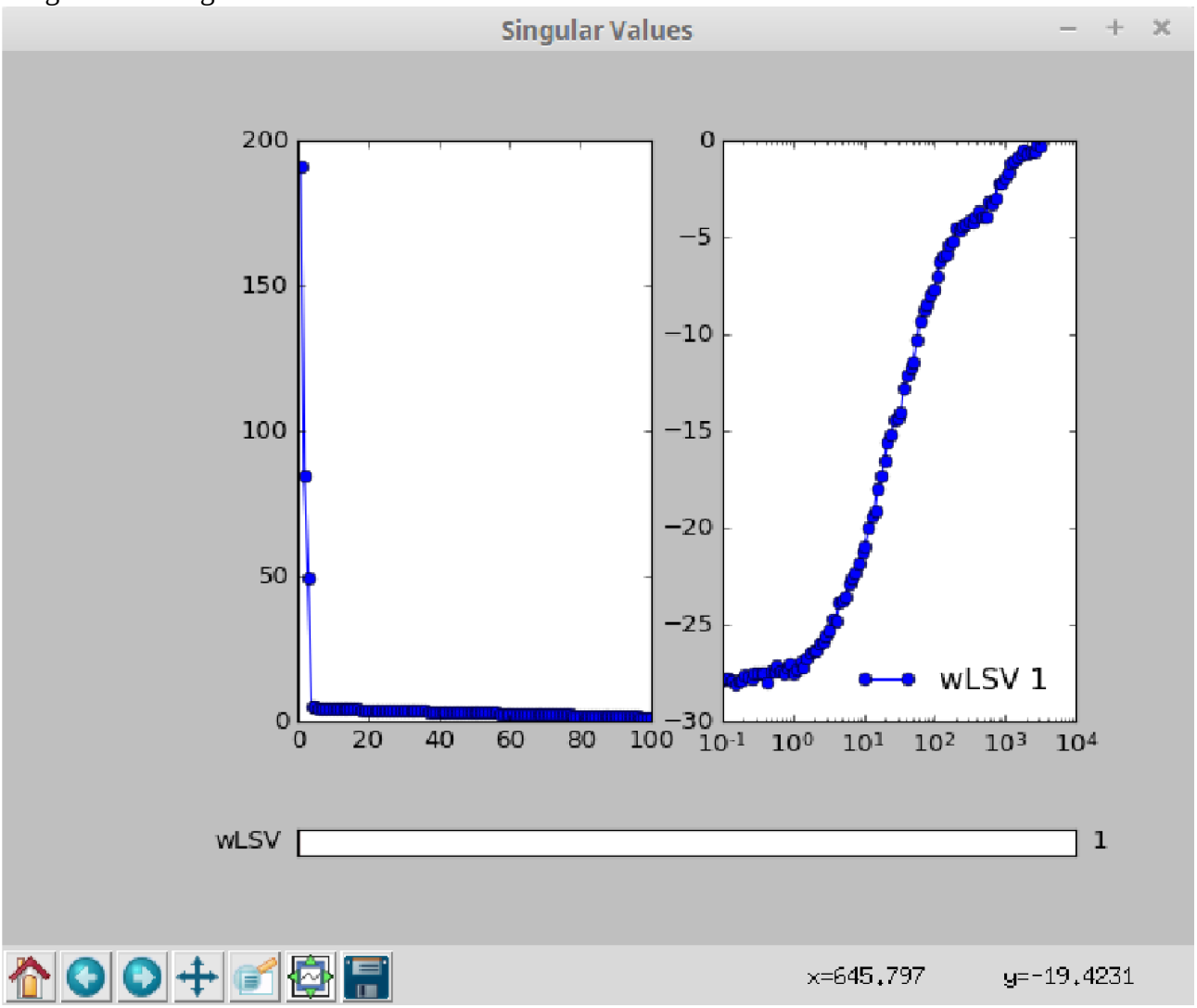
2. When the data is loaded, it will be displayed on a symbolic lin-log plot. This means that a pseudo log scale will be used for negative time points. In addition, the plot will be linear between -1 and 1. Loading the file hettaus_noise10.csv from the Data subdirectory should display the following.



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.

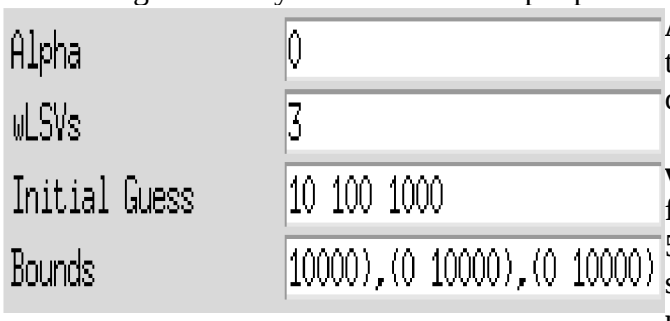
B

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



Note that the magnifying glass on the bottom tool panel allows you to zoom into the plot.

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. These are for hettaus_noise10.csv



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.

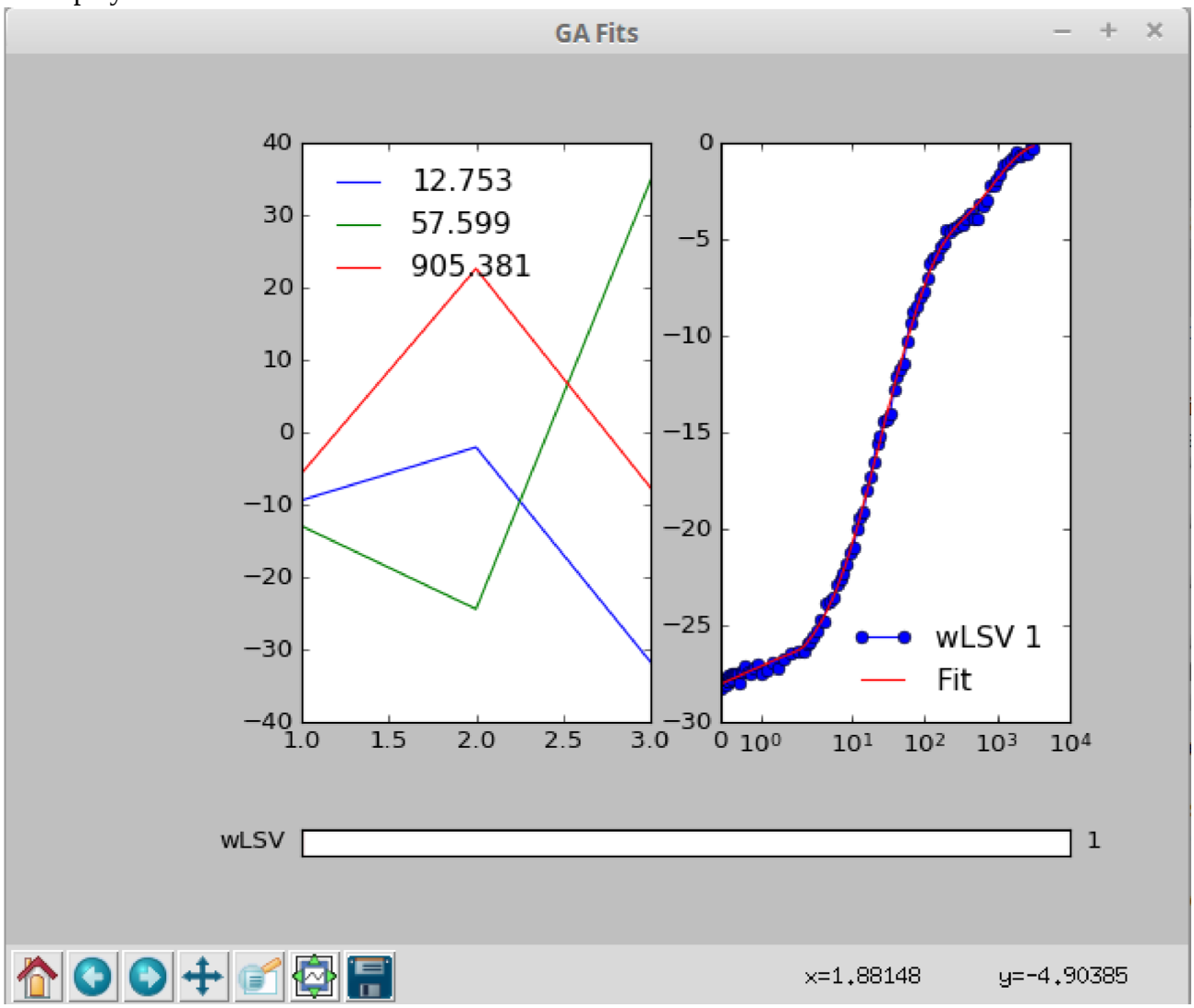
Bounds: Are fitting bounds for the non-linear solver. There must be a matching number of sets of bounds to number of guesses. The bounds are entered in the following format: (lower_bound upper_bound),(lower_bound2 upper_bound2),... with spaces separating the lower and upper bound for a single lifetime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

The settings for the fulldata_noise10.csv and dynamic_noise10.csv respectively are:

Alpha	0
wLSVs	5
Initial Guess	5 10 50 500 5000
Bounds	10000),(0 10000),(0 10000

Alpha	0
wLSVs	1
Initial Guess	60
Bounds	(0 10000)

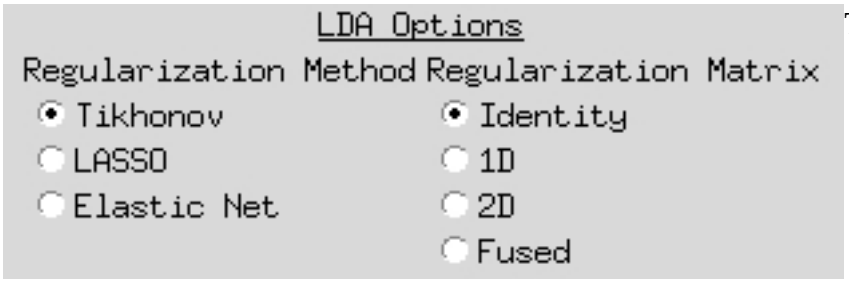
3. Using those values as initial parameters for the hettaus_noise10, the following results screen will be displayed:



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.



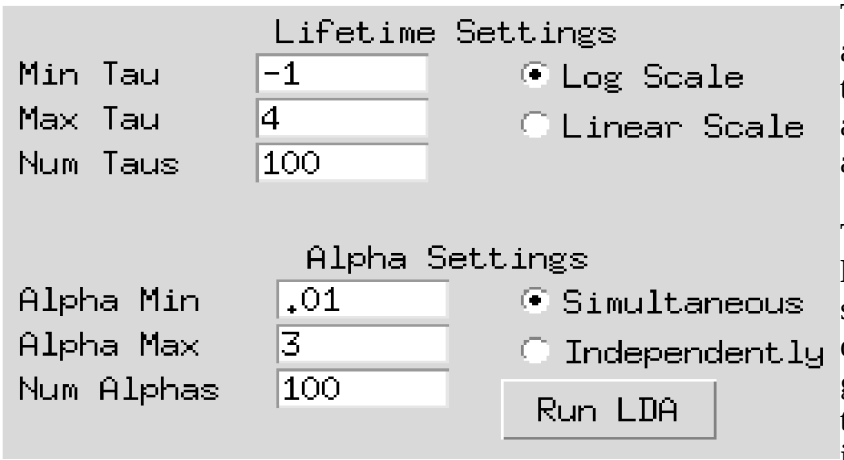
The matrices are as follows:

- Identity is simply an identity matrix
- 1D is a first derivative approximation $\frac{1}{2}\begin{bmatrix} 1 & -1 & 0 & & \cdots \\ 0 & 1 & -1 & 0 & \cdots \\ 0 & 0 & 1 & -1 & \cdots \end{bmatrix}$
- 2D is a second derivative approximation: $\frac{1}{4}\begin{bmatrix} -2 & 1 & 0 & & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \end{bmatrix}$
- Fused is a combination of the identity and first derivative matrices:

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

D

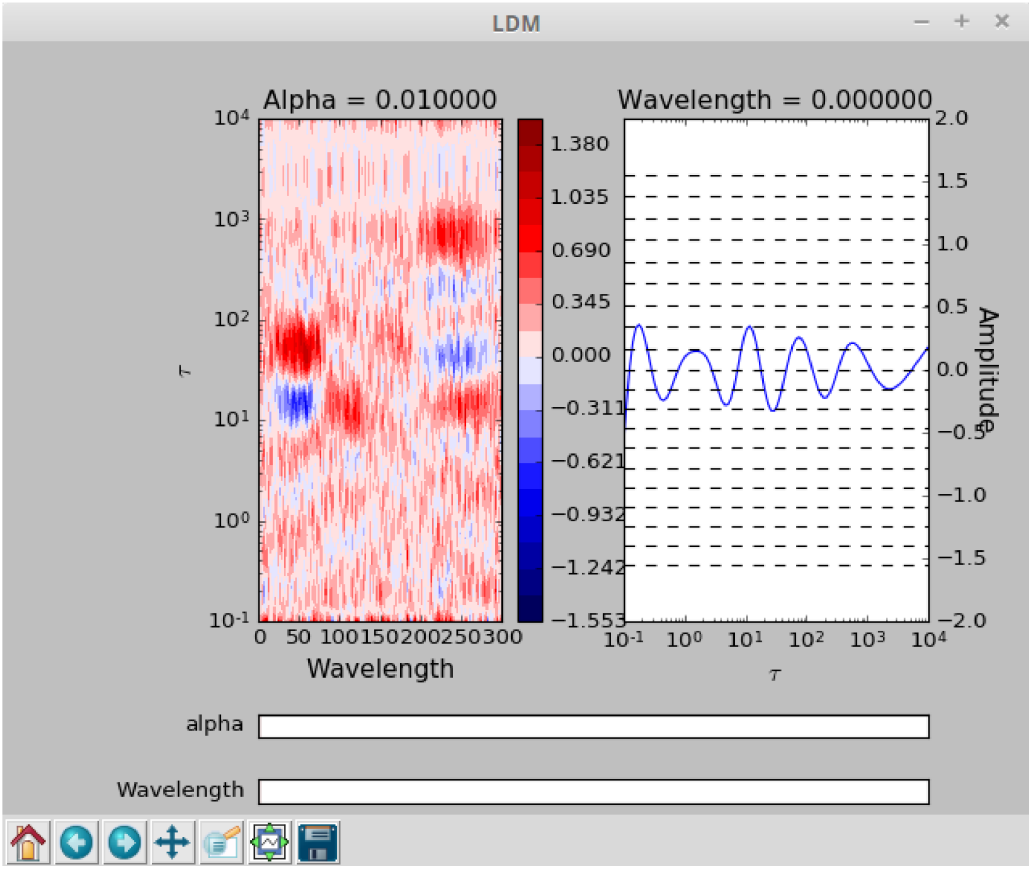
1. These settings determine the number and scale of your lifetimes, as well as the alpha selection parameters. Note that for elastic net, the rho values are simply distributed on a scale from 0 to 1 in tenths, in addition to any alpha values you select.



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}.

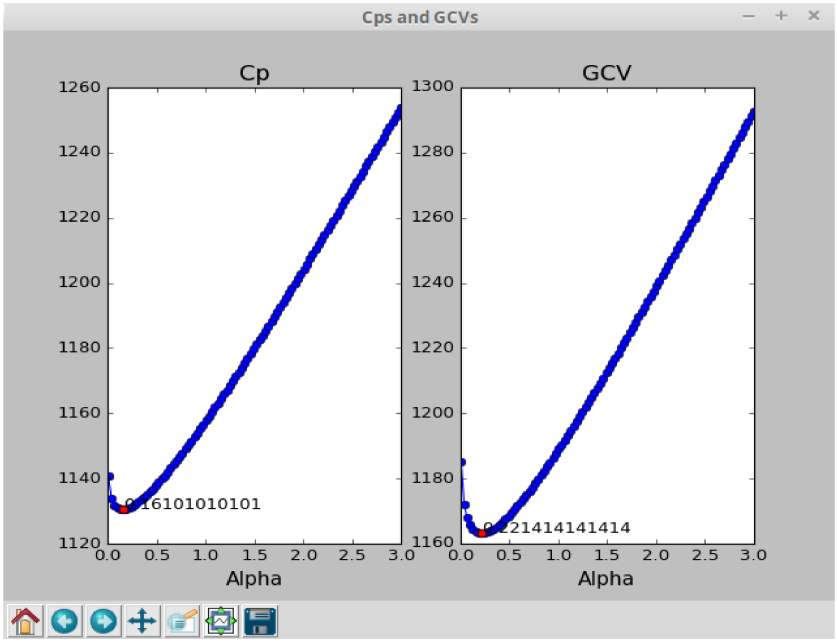
The alphas are distributed along a linear scale. The selection of simultaneous or independently determines whether statistics are generated for all wavelengths together (simultaneous) or each independently.

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.



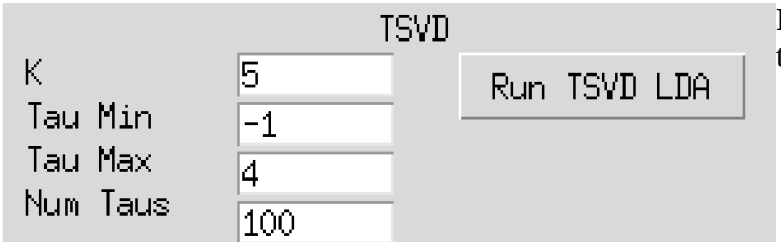
The alpha slider will allow you to slide through the LDMs produced at each alpha value. The right plot shows a single vertical slice through the LDM, at a particular wavelength. The wavelength slider allows you to look through the results at various wavelengths. The dashed lines represent the contour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

You will also see two windows corresponding to alpha selection statistics, like the following for GCV and Cp statistics.



E

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



K is the singular value at which to truncate the design matrix.

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**.

2. The replot contours button will reproduce an LDM, using the entered number of contour levels above and below zero.