

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 pyla.py` from the `pylda` directory.

The screenshot shows the PyLDA GUI with the following sections highlighted by red boxes and letters:

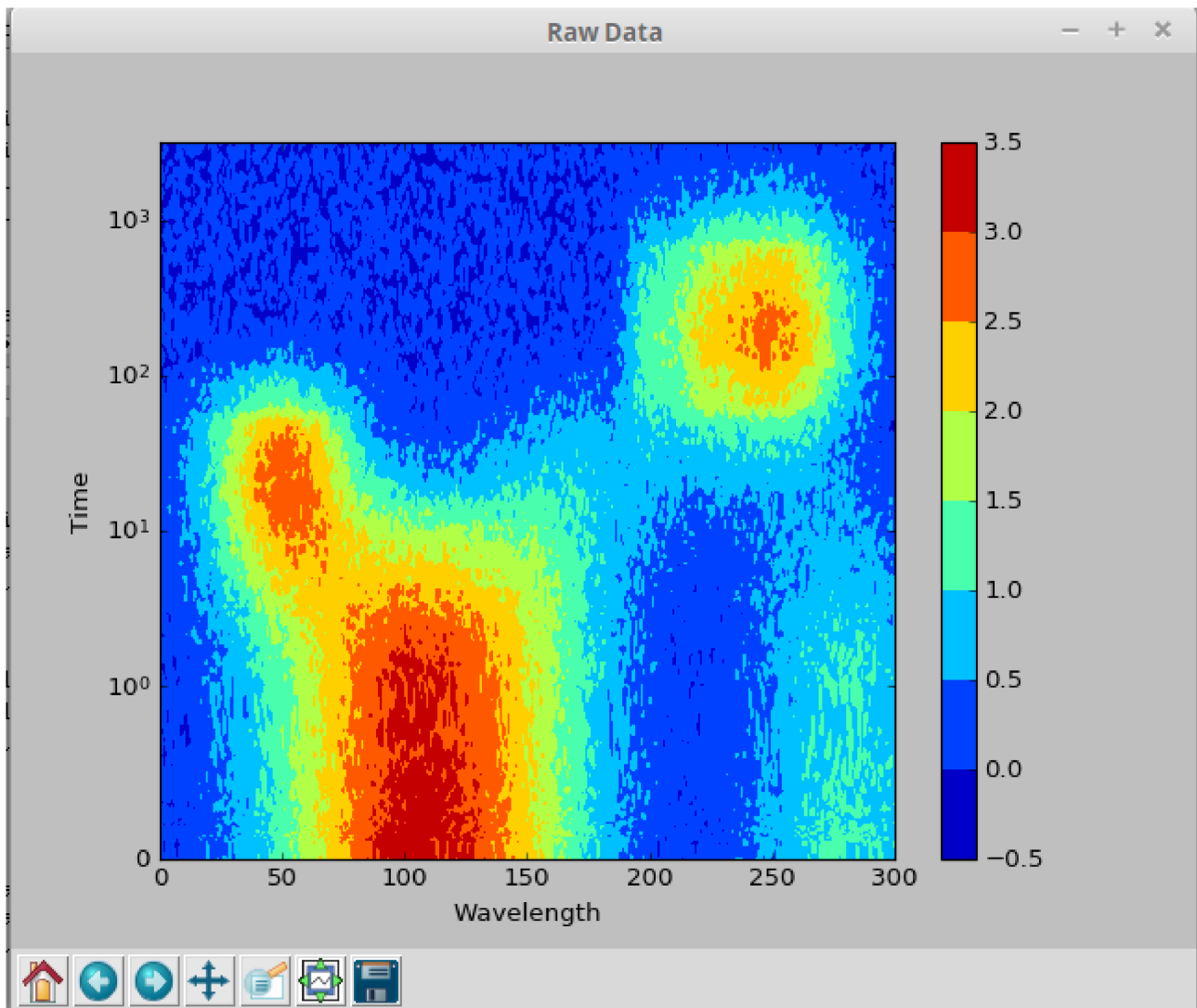
- A**: Top-left section containing a "Load File" button and "Time and Wavelength Bounds" input fields (Time Min, Time Max, WL Min, WL Max) with an "Update Bounds" button.
- B**: Top-right section containing "IRF and Chirp Parameters" (FWHM,  $\mu$ ,  $\lambda$ , Order) and buttons for "Fix Values" and "Fit IRF".
- C**: Middle-left section containing "LDA Options" with radio buttons for Regularization Method (Tikhonov, LASSO, Elastic Net) and Regularization Matrix (Identity, 1D, 2D, Fused).
- D**: Middle-left section containing "Lifetime Settings" (Min Tau, Max Tau, Num Taus) and "Alpha Settings" (Alpha Min, Alpha Max, Num Alphas) with radio buttons for Log Scale, Linear Scale, Simultaneous, and Independently, and a "Run LDA" button.
- E**: Bottom-left section containing "TSVD" parameters (K, Tau Min, Tau Max, Num Taus) and a "Run TSVD LDA" button.
- F**: Middle-right section containing "SVD and GA Options" (Alpha, wLSVs, Initial Guess, Bounds) with "SVD" and "GA" tabs, and a "Low Rank Data Approximation" section with a "Truncate" button, "Replot LDM" text, and a "Replot" button with a "Num Contours" input field set to 10.

## A

1. Data should be in absorbance format. The file should be a CSV with the following formatting:

,	Wavelength $\lambda_1$ ,	Wavelength $\lambda_2$ ,
<b>Time <math>t_1</math>,</b>	$\Delta(t_1, \lambda_1)$ ,	$\Delta(t_1, \lambda_2)$ ,
<b>Time <math>t_2</math>,</b>	$\Delta(t_2, \lambda_1)$ ,	$\Delta(t_2, \lambda_2)$ ,

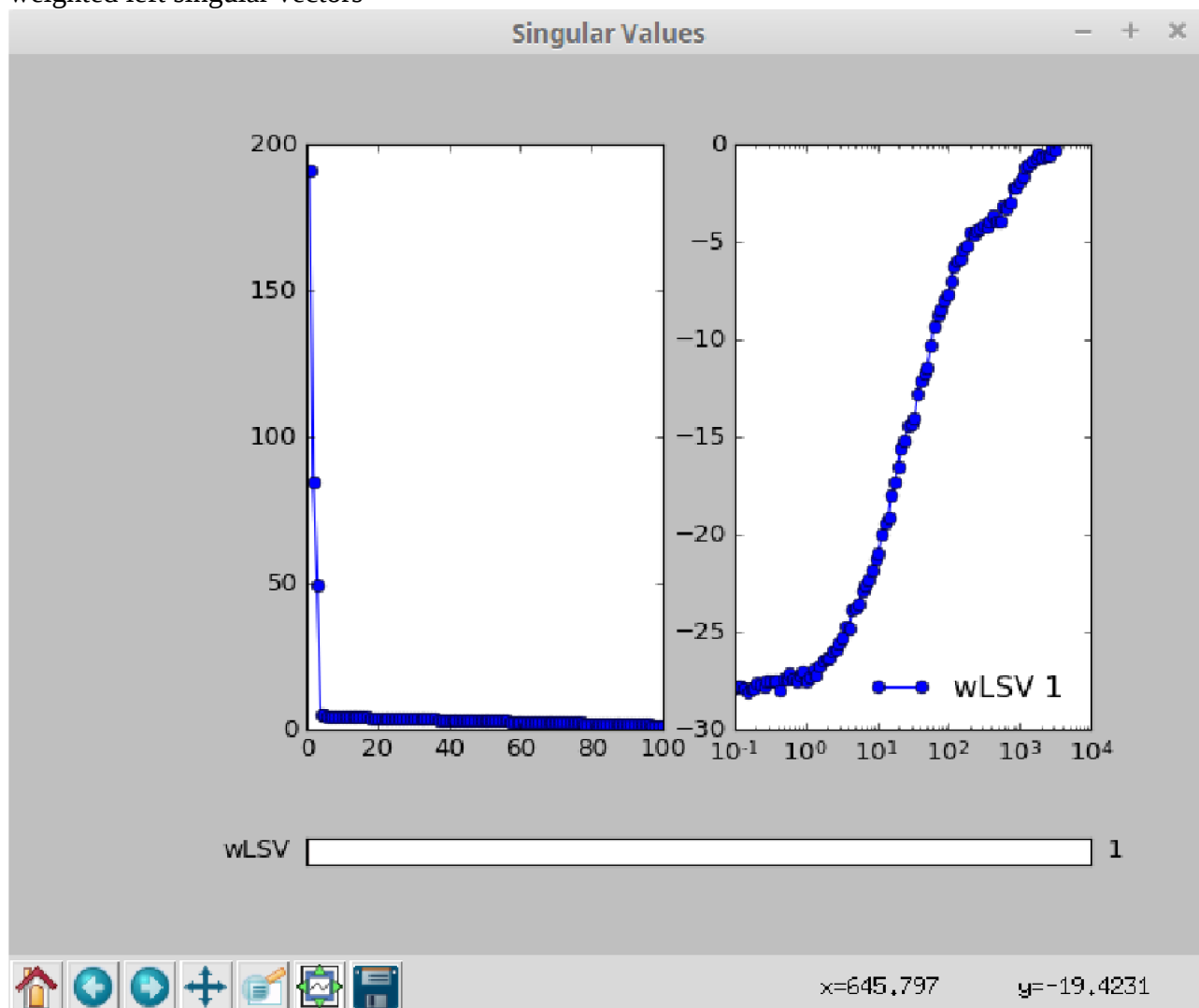
2. When the data is loaded, it will be displayed on a symbolic lin-log plot. This means that a pseudo log scale will be used for negative time points. In addition, the plot will be linear between -1 and 1. Loading the file `hettaus_noise10.csv` from the Data subdirectory should display the following.



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	0	<b>Alpha:</b> will allow Tikhonov regularization if set to a value other than 0. By default it is 0, corresponding to an ordinary least-squares
wLSVs	3	
Initial Guess	10 100 1000	<b>wLSVs:</b> 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
Bounds	10000),(0 10000),(0 10000)	

**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.

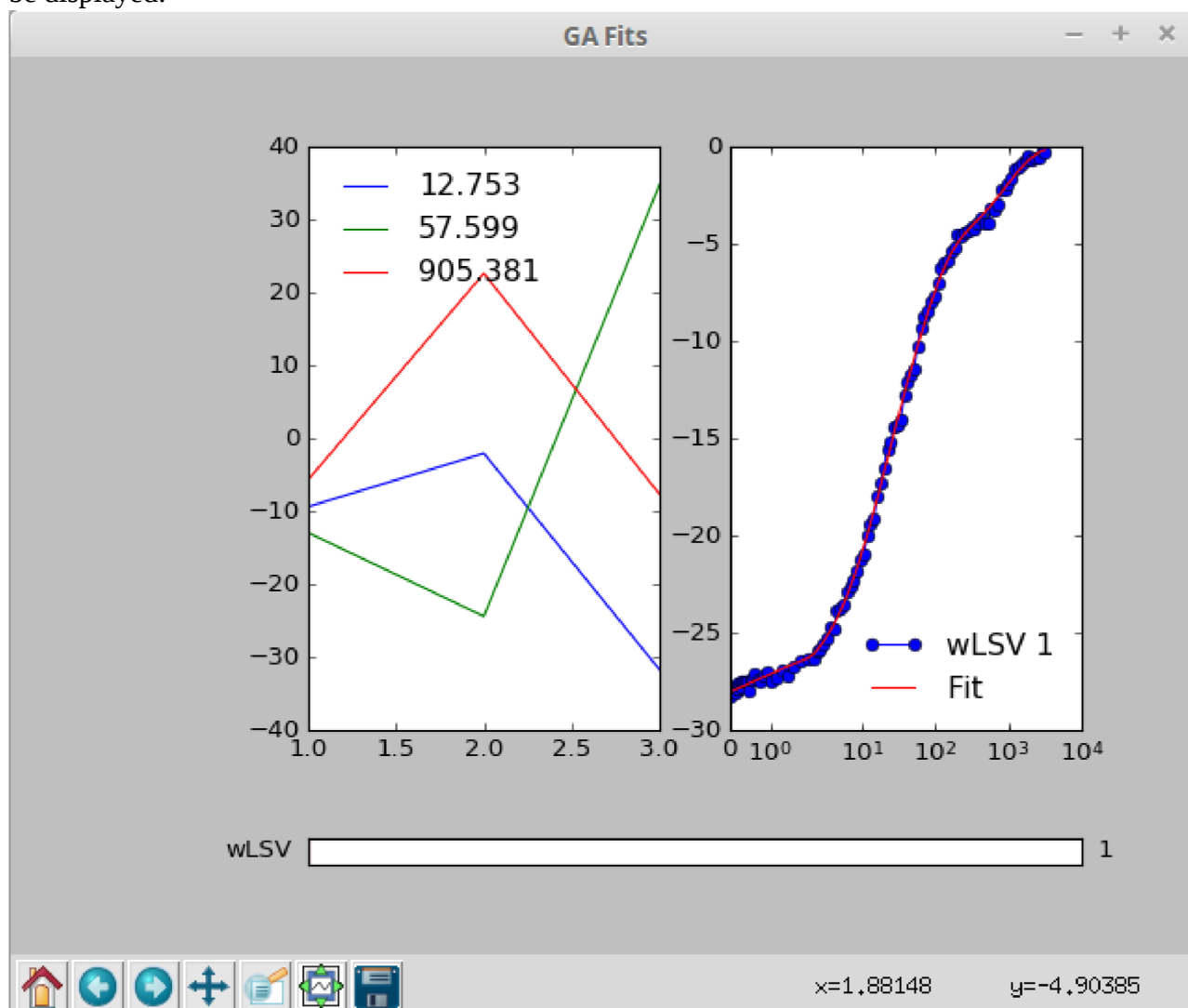
**Bounds:** Are fitting bounds for the non-linear solver. There must be a matching number of sets of bounds to number of guesses. The bounds are entered in the following format: (lower\_bound upper\_bound),(lower\_bound2 upper\_bound2),... with spaces separating the lower and upper bound for a single 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.

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

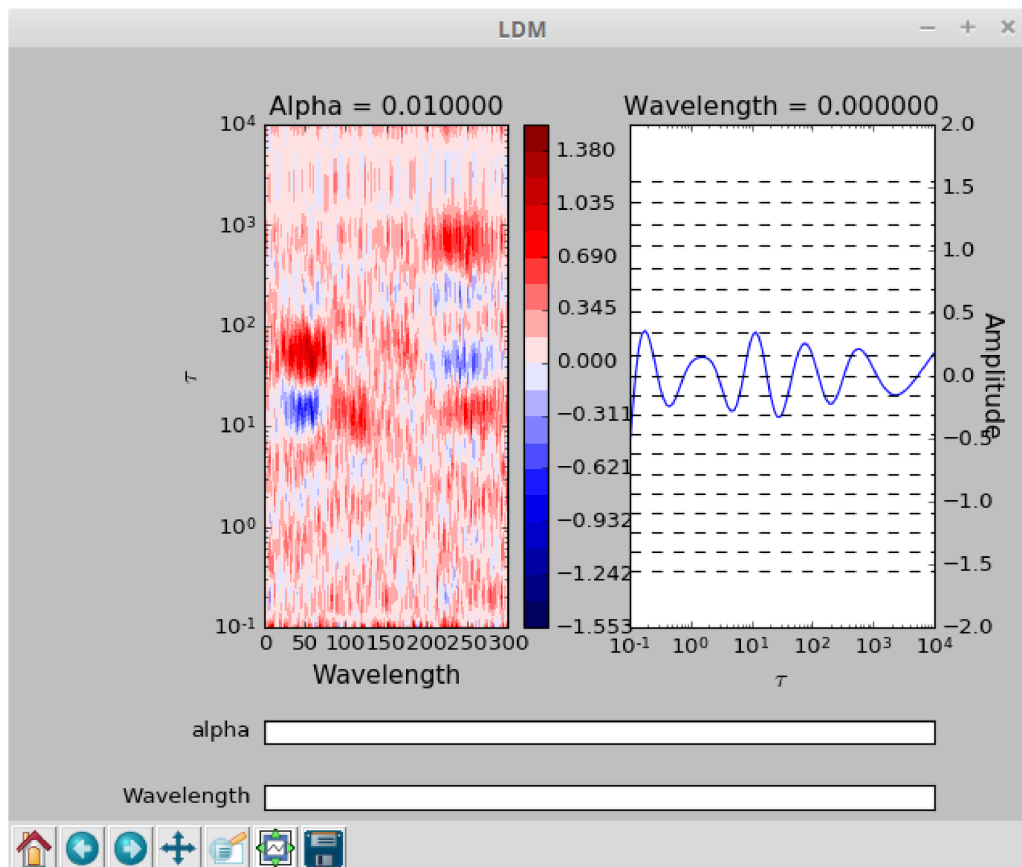
Alpha Settings		
Alpha Min	<input type="text" value=".01"/>	<input checked="" type="radio"/> Simultaneous
Alpha Max	<input type="text" value="3"/>	<input type="radio"/> Independently
Num Alphas	<input type="text" value="100"/>	

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.

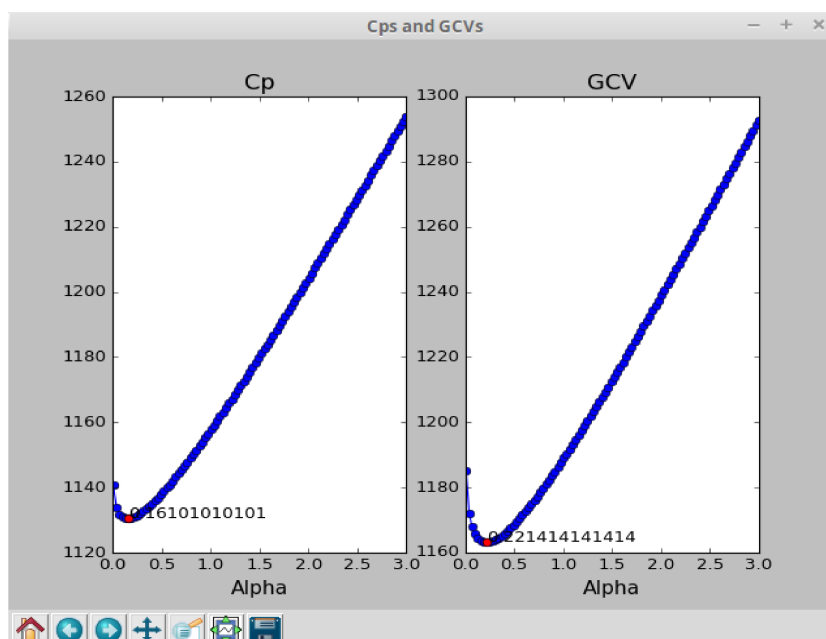
2. Run LDA will produce a LDM like the following:

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.

TSVD	
K	<input type="text" value="5"/>
Tau Min	<input type="text" value="-1"/>
Tau Max	<input type="text" value="4"/>
Num Taus	<input type="text" value="100"/>

Run TSVD LDA

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.