Phys 512 PS4

Andrew Lewis

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a)

The analytical derivatives of our lorentzian are as follows:

$$\frac{dy}{da} = \frac{1}{1 + (t - t0)^2/w^2}$$

$$\frac{dy}{dt0} = \frac{2.0 * a/w^2 * (t - t0)}{(1 + (t - t0)^2/w^2)^2}$$

$$\frac{dy}{dw} = \frac{2 * a * (t - t0)^2}{w^3 * (((t - t0^2)/w^2 + 1)^2}$$

and the guess for the values of parameters are:

$$a = 1.423$$

$$t0 = 1.925358e - 4$$

and

$$w = 1.7924e - 5$$

approximately This plot looked like:

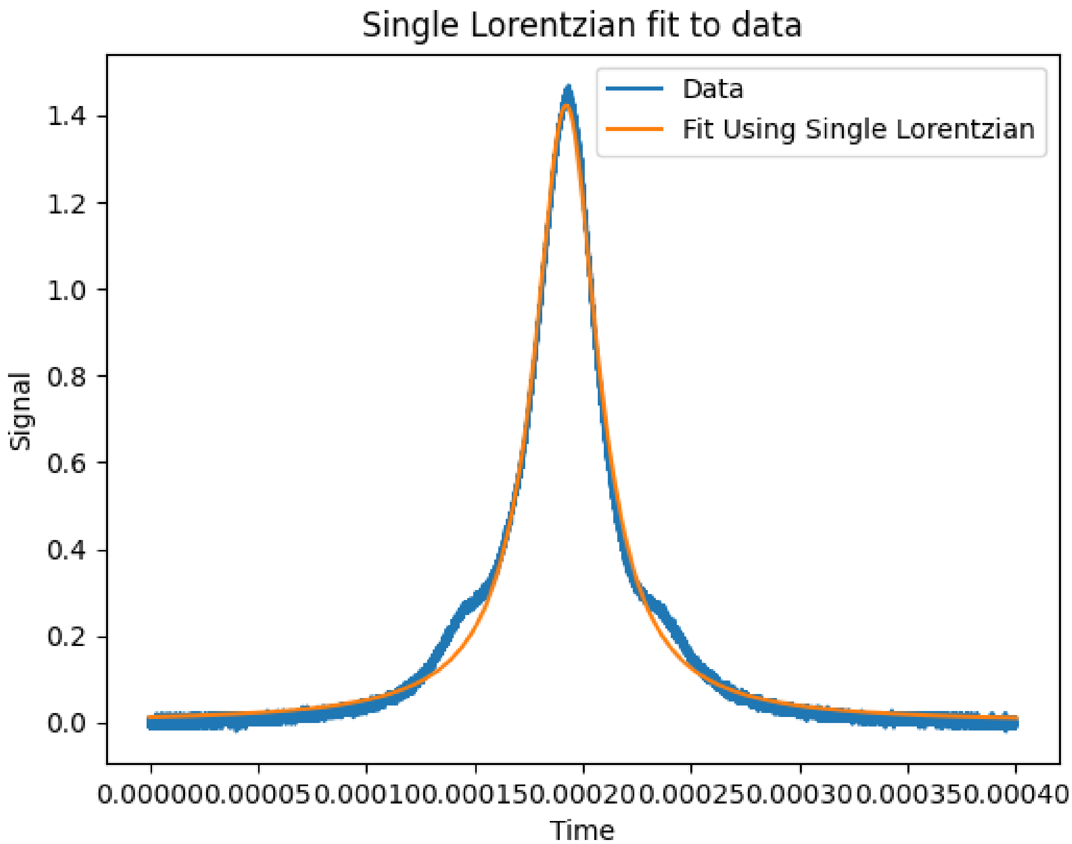

Figure 1: Fit of our data using Newton's method and analytical derivatives

b)

We are going to assume that the noise is gaussian uniformly distributed- therefore we can take the noise in our data to be

$$n = dTrue - d$$

then to get the average noise we will just take the standard deviation (sans error bars)

$$averageNoise = std(dTrue - d)$$

Then we can find the error in the parameters using the formula from class

$$covariance = (A.T@N^{-1}@A)^{-1}$$

where the diagonals in our N matrix is our error in our data points which will all be the same. The estimated errors in our parameters are

$$a = 4.22291326e - 04$$

$$t0 = 5.31820045e - 09$$

$$w = 7.53124668e - 09$$

c)

Now we are supposed to do the same thing as part A but use numerical derivatives. Using numerical derivatives the answers for our parameters are:

$$a = 1.4234$$

$$t0 = 1.92251581e - 04$$

$$w = 1.79081219e - 05$$

Which are all very close, usually to within a 1000th of the analytical errors. This could be improved with an error tolerance.

$$\boxed{\text{They were not significantly different from the analytical derivatives}}$$

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d)

We were able to generalize our numerical differentiator to a 6 parameter function, and then use it to find parameters for the the 3 peaked loretzian.

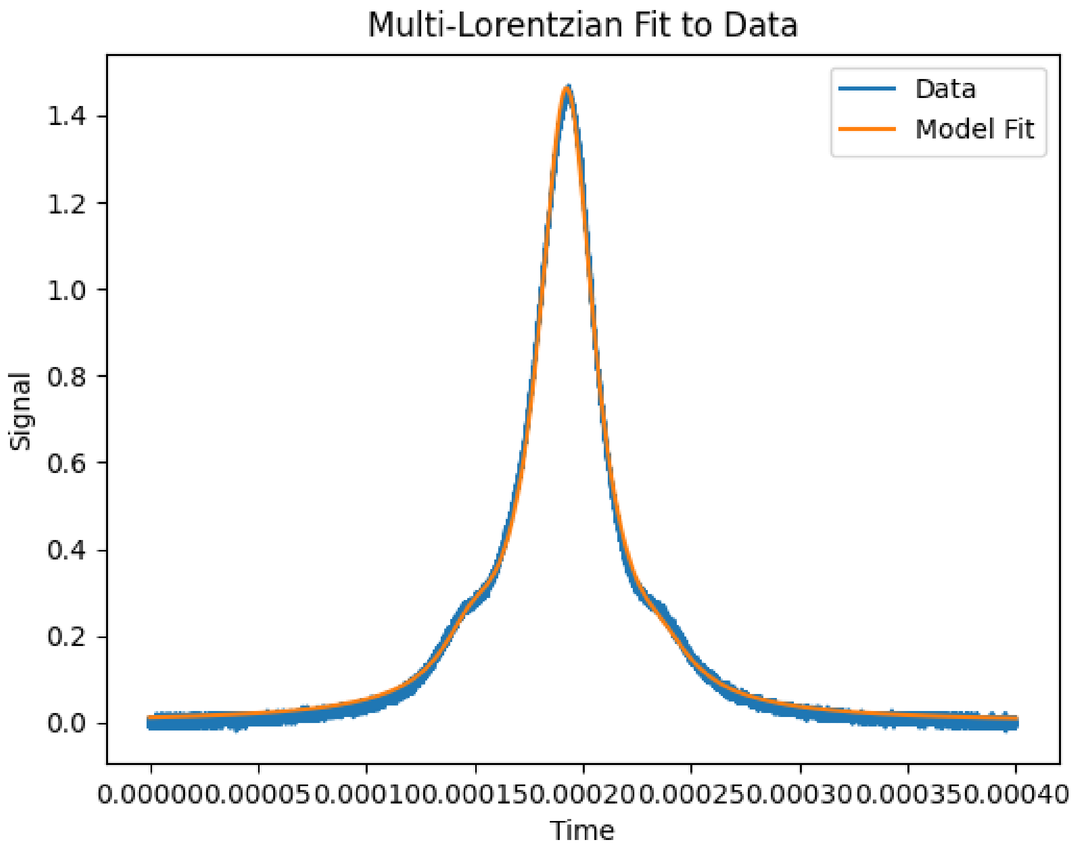

Figure 2: Fit of model to data using 3 lorentzians. As is evident in the figure, the model with 3 peaks does a better job of picking up the symmetrical off center features.

The estimates on the parameters were:

$$a = 1.4429920621045567$$
$$b = 0.06473185228998703$$
$$c = 0.1039102997403473$$
$$t0 = 0.00019257785145156235$$
$$w = 1.6065128537024153e - 05$$
$$dt = -4.456728541127008e - 05$$

and the errors were calculated in the same way as b

$$\delta a = 2.32683195e - 04$$
$$\delta b = 2.17305659e - 04$$
$$\delta c = 2.21928768e - 04$$
$$\delta t0 = 2.75490861e - 09$$
$$\delta dw = 4.93373033e - 09$$
$$\delta dt = 3.32108595e - 08$$

e)

Look at the residuals.
The residuals are as follows:

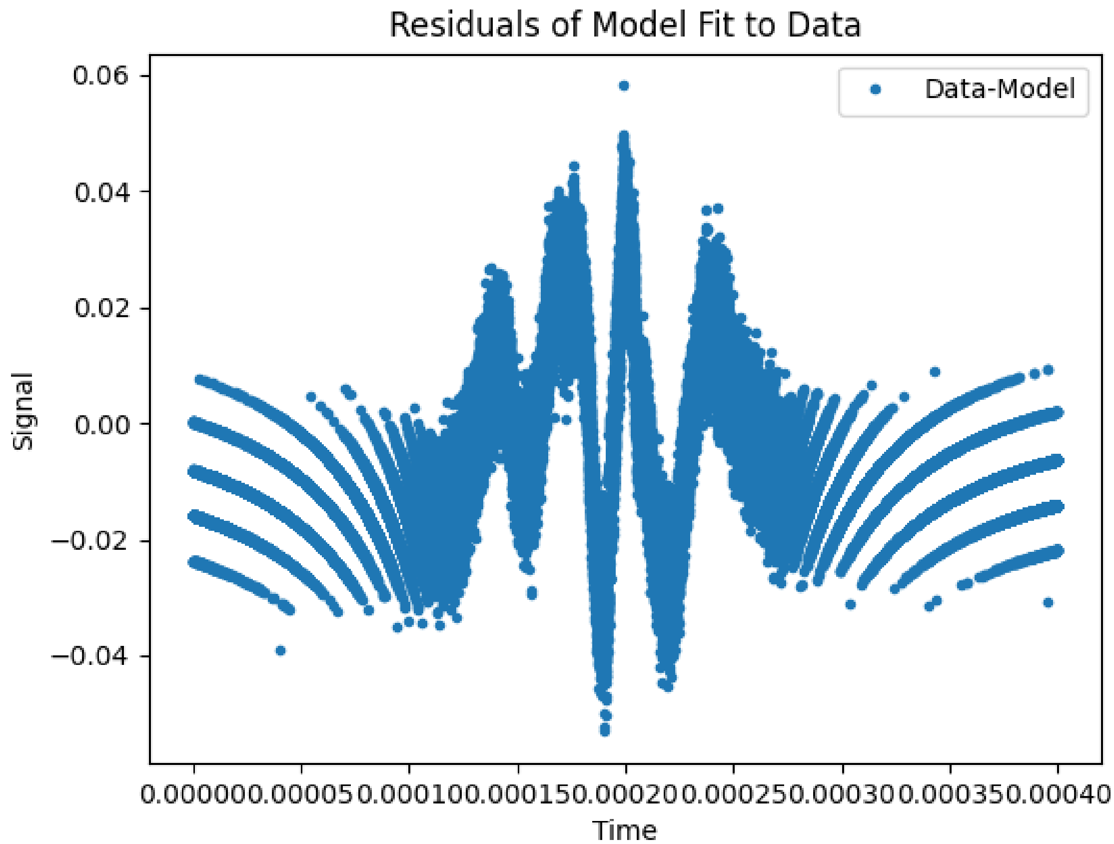

Figure 3: Residuals of the multilorentzian and the data.

As can be seen in the residuals there is still a distinct pattern in the data. Therefore I would say that it is not fair to assume that the errors and data are independent and our model is not a complete description of the data.

$$\boxed{\text{There are unaccounted for variables/ correlations in the data/model}}$$

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f

The plot i get from adding the parameter errors to the parameters is: The two chi squares we got were:

$$\text{Optimal Parameters} = 509.88497405082944$$

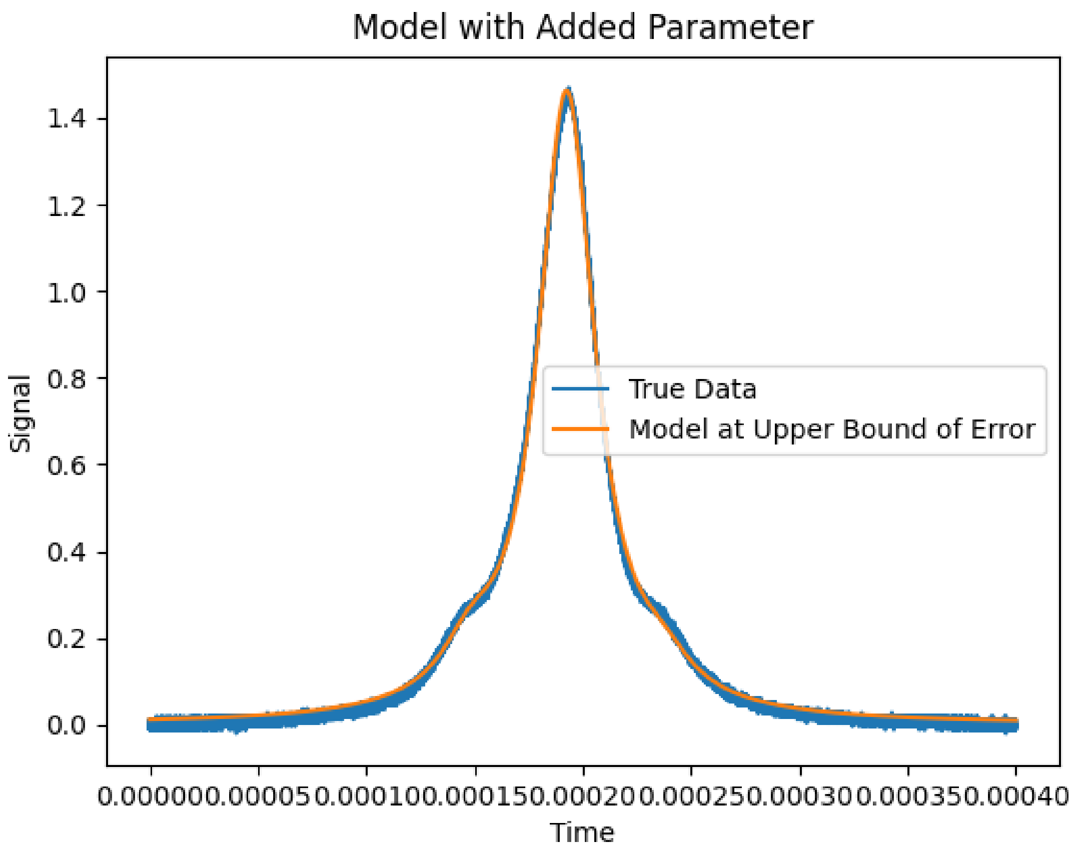

Figure 4: Model fit of the parameters + parameter errors

and

$$\text{Shifted} = 510.8524370952099$$

They are almost identical- this is to be expected as it is within the errors of all the parameters. But the shifted one will be a bit higher as it is less of a good fit for the data.

g)

Redo the fit using an MCMC First off does our chain converge?

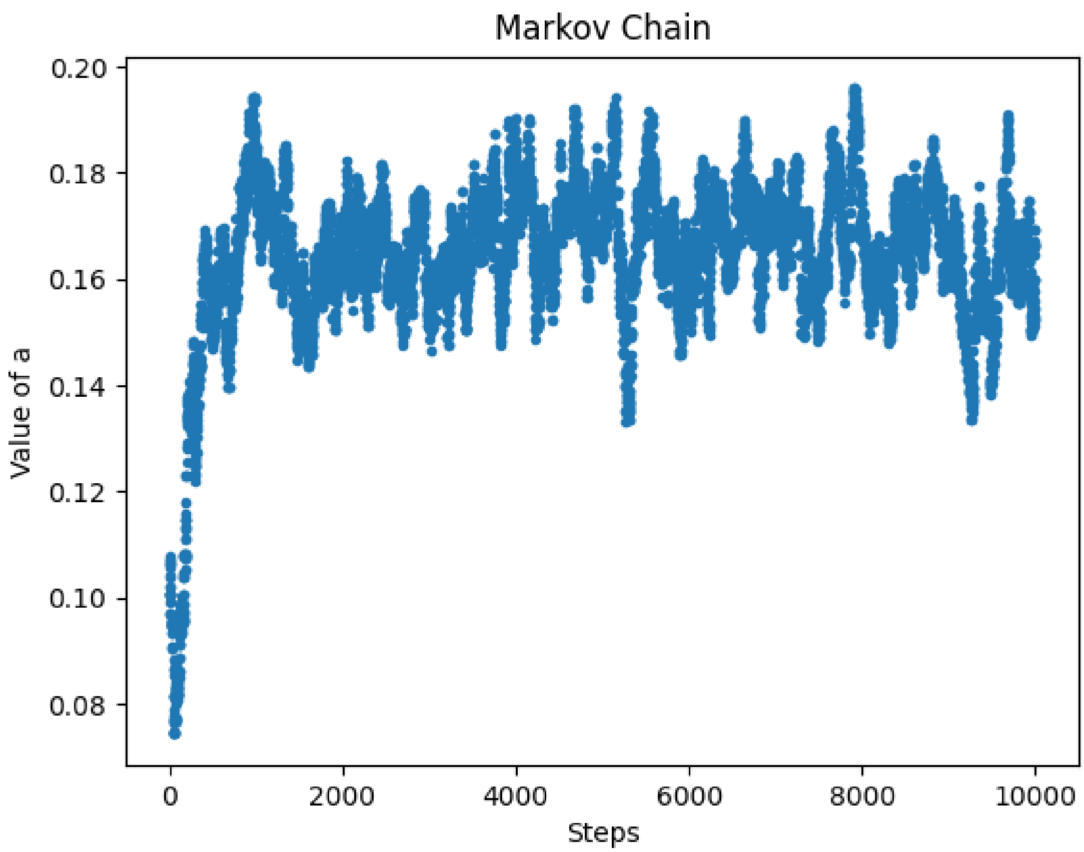

Figure 5: Showing the MCMC chains

from the above figure it is obvious that the chain converges. And the parameters produced a plot that looked like:

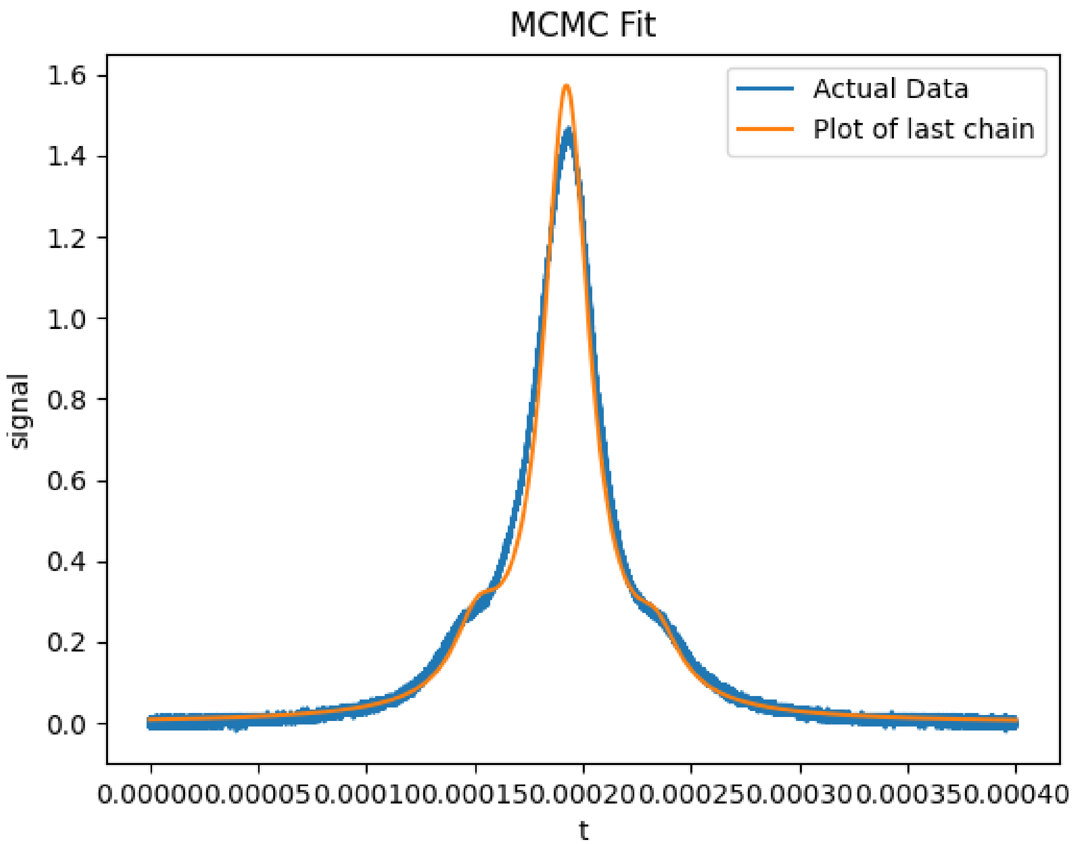

Figure 6: Best fit MCMC plot

the best fit parameters ended up being:

$$a = 1.545$$

$$b = 0.1358$$

$$c = 0.16654458496221597$$

$$t0 = 0.00019253757563655338$$

$$w = 1.3036185830694659e - 05$$

$$dt = -4.1307424795474976e - 05$$

and the errors were larger- turning into

$$\delta a = 0.021179421019835398$$

$$\delta b = 0.009653883432921041$$

$$\delta c = 0.009691022573984886$$

$$\delta t0 = 1.9251325865918842e - 07$$

$$\delta w = 1.6878084413410064e - 07$$

$$\delta dt = 9.03865504111868e - 07$$

h)