## Subject: doubt in chisq value Posted by sid on Mon, 01 Nov 2010 06:43:15 GMT

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Hi,

I am fitting my data with svdfit (2 degree polynomial), now I need to know how exactly the chisq value is calculated in this routine, because I need to know the goodness of fit. For my data which I am fitting I am getting chisq values which varies from 6.3534419e-07 to 8.0278877e-09 for different datasets. But please help how the routine is performing the chisq calculation and how can I find the goodness of fit from it. thanking you sid

Subject: Re: doubt in chisq value Posted by David Gell on Tue, 02 Nov 2010 14:59:05 GMT View Forum Message <> Reply to Message

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On Nov 2, 2:29 am, sid <gunvicsi...@gmail.com> wrote:
> On Nov 1, 7:48 pm, wlandsman <wlands...@gmail.com> wrote:
>
>
>> On Nov 1, 2:43 am, sid <gunvicsi...@gmail.com> wrote:
>
>>> Hi,
       I am fitting my data with svdfit (2 degree polynomial), now I need
>>> to know how exactly the chisq value is calculated in this routine.
>>> because I need to know the goodness of fit. For my data which I am
>>> fitting I am getting chisq values which varies from 6.3534419e-07 to
>>> 8.0278877e-09 for different datasets. But please help how the routine
>>> is performing the chisq calculation and how can I find the goodness of
>>> fit from it.
>>> thanking you
>>> sid
>> You are almost certainly supplying unrealistic error bars (sigma
>> values).
>> Chisq can be calculated from the single line (e.g. see curvefit.pro)
>
>> chisq = total(Weights*(y-yfit)^2)/nfree
>> where weights = 1/sigma^2, and nfree is the number of data points
>> minus the number of free parameters.
>> --Wayne
```

>

- > Does the sigma value denote the error in each y value? If so can you
- > suggest me how to find the error for each y value, mine is a spectral
- > data. I am fitting a spectral line with 2 degree polynomial.
- > thanking you
- > sid
- > sid

You seem to be asking some very basic questions about the propagation of errors and data reduction. I would suggest you check out the textbook "Data Reduction and Error Analysis for the Physical Sciences" by Bevington and Robinson. Chapter 1, "Uncertainties in Measurements", chapter 3 "Error Analysis" and chapter 11, "Testing the Fit" discuss the questions you are asking.

As far as determining the error (precision is a better term) in each y value, that depends to a certain extent on how the data is collected. If you don't know how the data is collected, use the same value of sigma for each measurement, which is equivalent of stating that all of the measurements are equally good. If the spectra is obtained using a counting detector, you might use sqrt(Yn) for sigma(Yn), Poisson statistics. If your spectra is obtained by an analog device, measuring say current, you might use a fraction of the signal as the measurement error.

If you are trying to fit a function to a spectral line, a polynomial may not be a good choice, unless you limit the data to a few points around the peak. Better choices might be a Gaussian or Lorentzian. The Lorentzian will model a spectra line with wings. Both line shapes have 3 parameters, a center, width and amplitude. If you are modeling a composite spectra, you can use a sum of Gaussians, each with different parameters.