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Subject: Problems in non-linear fitting

Posted by [duxiyu@gmail.com](mailto:duxiyu@gmail.com) on Thu, 15 Mar 2007 09:04:12 GMT

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I am using the MPFITFUN for curve-fitting.  
It is easy and effectual.  
But I have some confused points in using it.

Could it give a value which can measure the quality of fitting?

For example, if you do a linear fitting, you can calculate the  $R^2$  to measure the quality of fitting.

This R maybe is the correlate coefficient between Y and Yfit. (I am not sure for this. if you know how the R is calculated, please tell me.)

I do not know whether the  $R^2$  can describe the quality of non-linear fitting.

Because when I select the different starting values of the parameters to fit, I get the different results, I need a parameter to determine which result is best.

If it not, I want to find a new parameter which can meet my request.

Best regards,  
Du Jian

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Subject: Re: Problems in non-linear fitting

Posted by [Vince Hradil](#) on Thu, 15 Mar 2007 15:25:54 GMT

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On Mar 15, 4:04 am, "dux...@gmail.com" <dux...@gmail.com> wrote:

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> Best regards,

> Du Jian

Read the "header" of the mpfitfun.pro file. Especially look for the  
PERROR keyword.

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Subject: Re: Problems in non-linear fitting  
Posted by [Craig Markwardt](#) on Thu, 15 Mar 2007 15:30:23 GMT  
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"duxiyu@gmail.com" <duxiyu@gmail.com> writes:

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- > It is easy and effectual.
- > But I have some confused points in using it.
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- > Could it give a value which can measure the quality of fitting?
- > For example, if you do a linear fitting, you can calculate the  $R^2$  to
- > measure the quality of fitting.
- > This R maybe is the correlate coefficient between Y and Yfit. (I am not
- > sure for this. if you know how the R is calculated, please tell me.)
- > I do not know whether the  $R^2$  can describe the quality of non-linear
- > fitting.

R does not necessarily measure the quality of fit, but rather the  
degree of \*linear\* correlation between two variables. Thus, it is  
only appropriate for linear fitting.

The  $\chi^2$  statistic is more commonly used for non-linear fitting; see  
the BESTNORM parameter of MPFIT & MPFITFUN.

- > Because when I select the different starting values of the parameters
- > to fit, I get the different results, I need a parameter to determine
- > which result is best.
- > If it not, I want to find a new parameter which can meet my request.

You may be getting different solutions for two different reasons that  
I can think of. One possibility is that there are multiple local  
minima. In that case, MPFIT is not the best method; perhaps monte  
carlo or simulated annealing would be more appropriate.

Another possibility is that you are using the automatic derivatives,  
but MPFIT is varying the parameters by too little to calculate an  
accurate derivative. In that case you should use the PARINFO  
parameter with the STEP or RELSTEP fields, to declare a step size to  
use for derivatives.

Good luck,  
Craig

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Craig B. Markwardt, Ph.D.    EMAIL: craigmnet@REMOVEcow.physics.wisc.edu  
Astrophysics, IDL, Finance, Derivatives | Remove "net" for better response  
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