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Subject: Re: mpfit and analytical derivative debugging

Posted by on Tue, 08 May 2012 13:53:55 GMT

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Den tisdagen den 8:e maj 2012 kl. 15:04:24 UTC+2 skrev Mats Löfdahl:

> I have this fitting problem that I'm solving with mpfit. The code works but the function values are kind of costly to calculate and the penalty for calculating the analytical derivatives once you have calculated the function value is relatively small. So I'm trying to use the AUTODERIVATIVE=0 setting.

>

> I've tested my analytical derivatives against numerical derivatives in a standalone program that does not involve mpfit. Looks fine.

>

> However, there seems to be something wrong because the problem does not converge anymore. (The solution does not change significantly from one iteration to the next.) Most likely an order of magnitude problem because the problem does not go away when I change the sign of the derivatives. (Or something more fundamental that I've misunderstood.)

>

> So I'm setting

>

```
>         parinfo[iparam].mpderiv_debug = 1
>         parinfo[iparam].mpderiv_reltol = 1d-3
>         parinfo[iparam].mpderiv_abstol = 1d-7
```

>

> for all parameters, expecting screen output of this sort (from doc header of mpfit.pro):

>

```
> ; FJAC DEBUG BEGIN
> ; #   IPNT   FUNC  DERIV_U  DERIV_N  DIFF_ABS  DIFF_REL
> ; FJAC PARM 2
> ;      80 -0.7308  0.04233  0.04233 -5.543E-07 -1.309E-05
> ;      99  1.370  0.01417  0.01417 -5.518E-07 -3.895E-05
> ;     118  0.07187 -0.01400 -0.01400 -5.566E-07  3.977E-05
> ;     137  1.844 -0.04216 -0.04216 -5.589E-07  1.326E-05
> ; FJAC DEBUG END
```

>

> But what I get looks like this:

>

>

```
> FJAC DEBUG BEGIN
> #   IPNT   FUNC  DERIV_U  DERIV_N  DIFF_ABS  DIFF_REL
> # FJAC_MASK = 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
> analytical derivatives
> Iter    1 -- CHI-SQUARE =    328.57185 -- DOF = 65515
```

>

>

>

> The "analytical derivatives" line is just a printout from my MYFUNC indicating that it has entered the part where the analytical derivatives are calculated. I don't know how to interpret FJAC\_MASK

and the "Iter 1..." line shows that mpfit thinks it is done with this iteration.

>  
> Suggestions?  
>  
> /Mats

Oh, silly me! You must turn on the analytical derivatives using `parinfo.mpside=3` and not with `autoderivative=0` for the debugging to work.

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Subject: Re: mpfit and analytical derivative debugging  
Posted by [Craig Markwardt](#) on Tue, 08 May 2012 14:50:05 GMT  
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On Tuesday, May 8, 2012 9:53:55 AM UTC-4, Mats Löfdahl wrote:

> Den tisdagen den 8:e maj 2012 kl. 15:04:24 UTC+2 skrev Mats Löfdahl:  
>> I have this fitting problem that I'm solving with mpfit. The code works but the function values are kind of costly to calculate and the penalty for calculating the analytical derivatives once you have calculated the function value is relatively small. So I'm trying to use the AUTODERIVATIVE=0 setting.  
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>> ;       99    1.370   0.01417   0.01417 -5.518E-07 -3.895E-05  
>> ;       118   0.07187  -0.01400  -0.01400 -5.566E-07  3.977E-05  
>> ;       137    1.844  -0.04216  -0.04216 -5.589E-07  1.326E-05  
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>> But what I get looks like this:  
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```

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>> #      IPNT      FUNC  DERIV_U  DERIV_N  DIFF_ABS  DIFF_REL
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>> /Mats
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> Oh, silly me! You must turn on the analytical derivatives using parinfo.mpside=3 and not with
> autoderivative=0 for the debugging to work.

```

Thanks for reminding me to document FJAC\_MASK. It's just telling you which parameters MPFIT expects explicit derivatives from your user function. All 1s indicates all parameters.

You always have to set MPSIDE=3; that's well documented. :-)

But you are right that AUTODERIVATIVE=0 confuses the derivative debugging feature. There are several layers of options there and it's difficult to make them behave properly and document it well. For the future I think this can be fixed.

Craig

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Subject: Re: mpfit and analytical derivative debugging  
 Posted by on Tue, 08 May 2012 17:29:12 GMT  
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Den tisdagen den 8:e maj 2012 kl. 16:50:05 UTC+2 skrev Craig Markwardt:

> On Tuesday, May 8, 2012 9:53:55 AM UTC-4, Mats Löfdahl wrote:

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```

That doesn't help you if you're like me and think you are smarter than the documentation...

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Subject: Re: mpfit and analytical derivative debugging  
Posted by on Wed, 09 May 2012 08:32:29 GMT  
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Den tisdagen den 8:e maj 2012 kl. 19:29:12 UTC+2 skrev Mats Löfdahl:  
> Den tisdagen den 8:e maj 2012 kl. 16:50:05 UTC+2 skrev Craig Markwardt:  
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>> You always have to set MPSIDE=3; that's well documented. :-)  
>  
> That doesn't help you if you're like me and think you are smarter than the documentation...

Actually, here is one instance where the documentation could be improved (in mpfit.pro header):

```
; The keyword setting AUTODERIVATIVE=0 always globally overrides the  
; individual values of PARINFO.MPSIDE. Setting AUTODERIVATIVE=0 is  
; equivalent to resetting PARINFO.MPSIDE=3 for all parameters.
```

It kind of suggests that I should have been able to do what I did.

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