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.
>>
>> 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 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.

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
