
Subject: mpfit and analytical derivative debugging

Posted by on Tue, 08 May 2012 13:04:24 GMT

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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
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
