Subject: Re: Trouble with MPFITFUN

Posted by Helder Marchetto on Wed, 11 Apr 2012 18:08:31 GMT

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```
On Wednesday, April 11, 2012 6:34:23 PM UTC+2, Helder wrote:
```

- > Hi,
- > I've been spending a bit too much time on this and I am wondering what is going wrong here.
- > I'm trying to fit using a step function broadened by a Gaussian.
- > The fitting function is:

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- > FUNCTION GaussStep, X, P
- > ;Calculate the broadening of a step function with:
- > ;P[0] = step position
- > ;P[1] = left value
- > P[2] = right value
- > ;P[3] = step width
- > PRINT, P
- > P[0] = (P[0] > MIN(X)) < MAX(X)
- > Y = DBLARR(N ELEMENTS(X))
- > LowIndeces = WHERE(X LT P[0], CountLow, COMPLEMENT = HighIndeces,

NCOMPLEMENT=CountHigh)

- > IF CountLow GT 0 THEN Y[LowIndeces] = P[1]
- > IF CountHigh GT 0 THEN Y[HighIndeces] = P[2]
- > Sigma=P[3]
- > nPts=10*Sigma+1.0
- > kernel=DINDGEN(nPts)-(nPts-1)/2.0
- > kernel=EXP(-kernel^2/(2.*sigma^2))
- > kernel/=TOTAL(kernel,/DOUBLE)
- > yconvol = CONVOL(Y,kernel,/EDGE_TRUNCATE)
- > RETURN, yconvol
- > END

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- > To test MPFITFUN I use the following code:
- > PRO TestFit
- > xData = DINDGEN(201)
- yData = DBLARR(201)+RANDOMU(SEED,201,/DOUBLE)*0.2-0.1
- > yData[150:200] += 1.0D
- > StParam = [148D,MIN(yData),MAX(yData),3D]
- > DataErr = DBLARR(N ELEMENTS(xData))+0.2D
- > Results = MPFITFUN('GaussStep', xData,yData, DataErr, StParam, STATUS=status, /quiet)
- > PLOT, xData, yData
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- > PRINT, 'Final Parameters = ', Results
- > PRINT, 'Start Parameters = ', StParam
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> The output shows all the calls of the fitting function. And I find that at the end there is always NO change in the first parameter. Here is an example of the output:

```
>
>
      148.00000
                 -0.099990073
                                 1.0994661
                                              3.0000000
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                                 1.0994661
                                              3.0000000
>
      148.00000
                 -0.099990071
                                 1.0994661
                                              3.0000000
>
      148.00000
                 -0.099990073
                                 1.0994661
                                              3.0000000
>
>
      148.00000
                 -0.099990073
                                 1.0994661
                                              3.0000000
      148.00000
                 0.0073445709
                                 1.0082363
                                              2.3488363
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      148.00000 -0.0039705287
                                 0.99188729
                                               2.0999998
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                                 0.99188729
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                                                  0.99188729
                                                                2.1000000
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                                                  1.0978406
                                                               3.0000000
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> Throughout all the fitting procedure the first parameter has never been changed.

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> I also tried playing with the XTOL parameter without any success.

> Any tips are appreciated.

> > Many thanks,

> Helder

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> PS: I tried lots of different initial conditions, I tried using "parinfo.fixed" to block the other parameters, ... but at the end I never get any change in P[0]... sigh..

> PSS: The function GaussStep is working fine... I can replot the data in the correct way by moving the parameters by hand.

Ok, just had some dinner and the head is a bit clearer now. I think everything is working fine. The only problem is that the square residuals don't change a lot when changing the position of the step. It's like finding the minimum on a flat 100 square meter surface with a little 1 square cm hole hidden somewhere...

I think this is it, if anybody has a suggestion on how to better estimate the step, that would be appreciated... I'll go for dessert and maybe get a good idea on how to do that.

Cheers, Helder

Subject: Re: Trouble with MPFITFUN Posted by Helder Marchetto on Wed, 11 Apr 2012 19:51:36 GMT

View Forum Message <> Reply to Message On Wednesday, April 11, 2012 8:08:31 PM UTC+2, Helder wrote: > On Wednesday, April 11, 2012 6:34:23 PM UTC+2, Helder wrote: >> Hi. >> I've been spending a bit too much time on this and I am wondering what is going wrong here. >> I'm trying to fit using a step function broadened by a Gaussian. >> The fitting function is: >> >> FUNCTION GaussStep, X, P >> ;Calculate the broadening of a step function with: >> ;P[0] = step position >>;P[1] = left value >> ;P[2] = right value >>; P[3] = step width >> PRINT, P >> P[0] = (P[0] > MIN(X)) < MAX(X)>> Y = DBLARR(N_ELEMENTS(X)) >> LowIndeces = WHERE(X LT P[0], CountLow, COMPLEMENT = HighIndeces, NCOMPLEMENT=CountHigh) >> IF CountLow GT 0 THEN Y[LowIndeces] = P[1] >> IF CountHigh GT 0 THEN Y[HighIndeces] = P[2] >> Sigma=P[3] >> nPts=10*Sigma+1.0 >> kernel=DINDGEN(nPts)-(nPts-1)/2.0 >> kernel=EXP(-kernel^2/(2.*sigma^2)) >> kernel/=TOTAL(kernel,/DOUBLE) >> yconvol = CONVOL(Y,kernel,/EDGE_TRUNCATE) >> RETURN, yconvol >> END >> >> To test MPFITFUN I use the following code: >> PRO TestFit >> xData = DINDGEN(201) >> yData = DBLARR(201)+RANDOMU(SEED,201,/DOUBLE)*0.2-0.1 >> yData[150:200] += 1.0D >> StParam = [148D,MIN(yData),MAX(yData),3D] >> DataErr = DBLARR(N_ELEMENTS(xData))+0.2D >> Results = MPFITFUN('GaussStep', xData,yData, DataErr, StParam, STATUS=status, /quiet) >> PLOT, xData, yData >> OPLOT, xData, GaussStep(xData,Results), COLOR = 255L >> PRINT, 'Final Parameters = ', Results >> PRINT, 'Start Parameters = ', StParam

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                  -0.099990071
                                   1.0994661
                                                3.0000000
>>
       148.00000
                                                3.0000000
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>> Any tips are appreciated.

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- >> Many thanks,
- >> Helder

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Ok, even dessert helped. By doing a smooth+deriv operations and then fitting the peak, I can get

quite reliably a peak.

I think I'll try to delete this post tomorrow and insert it in the hall of shame...

Cheers, h

Subject: Re: Trouble with MPFITFUN Posted by David Fanning on Wed, 11 Apr 2012 19:55:59 GMT

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Helder writes:

- > Ok, even dessert helped. By doing a smooth+deriv operations and then fitting the peak, I can get quite reliably a peak.
- > I think I'll try to delete this post tomorrow and insert it in the hall of shame...

Coyote was telling me they have pretty much run out of space in the current location. They are looking for an airport hanger, apparently, but won't be accepting new donations until they find something suitable. :-(

Cheers,

David

David Fanning, Ph.D.
Fanning Software Consulting, Inc.
Covered Civide to IDL Programmic

Coyote's Guide to IDL Programming: http://www.idlcoyote.com/

Sepore ma de ni thui. ("Perhaps thou speakest truth.")

Subject: Re: Trouble with MPFITFUN Posted by Craig Markwardt on Thu, 12 Apr 2012 05:10:08 GMT View Forum Message <> Reply to Message

On Wednesday, April 11, 2012 12:34:23 PM UTC-4, Helder wrote:

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ERF is much better than your convolution because it actually integrates the gaussian, rather than assuming that sampling a gaussian at a few discrete points is sufficient to integrate it.

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Best wishes, Craig Markwardt

Subject: Re: Trouble with MPFITFUN

Posted by Helder Marchetto on Thu, 12 Apr 2012 08:48:44 GMT

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On Thursday, April 12, 2012 7:10:08 AM UTC+2, Craig Markwardt wrote:

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                                               3.0000000
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      148.00000 -0.099990071
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```

```
148.00000
                 -0.099990073
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       148.00000 0.0073445709
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                                                2.3488363
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       148.00000 -0.0039705257
                                  0.99188729
                                                2.1000000
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- > Best wishes,
- > Craig Markwardt

Thanks Craig,

your tip was very useful. I never thought about the ERF! Here is the function I am now using:

FUNCTION StepErrFun, X, P ;Parameter definition ;P[0] = Step height ;P[1] = Location of step ;P[2] = 2*SQRT(ALOG(P[2])) is the FWHM ;P[3] = Step offset RETURN,(P[0]/2D)* ERFC((P[1]-X)/P[2])+P[3] END

So far it worked fine!

Thanks again.

I will see what I can do with the Parinfo parameters. I'm currently using the procedure to show live fitting whilst moving a cross section on an image and it seems stable enough... Fits edges also where one would not see one.

Regards, Helder

Subject: Re: Trouble with MPFITFUN Posted by Craig Markwardt on Thu, 12 Apr 2012 12:35:06 GMT View Forum Message <> Reply to Message

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                                                  2.1000000
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>> You are getting closer to the right track.

>>

>> If I were you, I would avoid complicated invocations of CONVOL. It looks like you can compute your "smoothed step function" exactly, by using the ERF (formerly ERRORF) function. I've used that before with success.

>>

>> ERF is much better than your convolution because it actually integrates the gaussian, rather than assuming that sampling a gaussian at a few discrete points is sufficient to integrate it.

>>

>> You might also want to play with using PARINFO, and setting the .STEP or .RELSTEP fields. The fitter can get stuck if your peak position and/or step position is between data samples. Set the parameter step size to something close to your data grid sample size.

>>

- >> Best wishes,
- >> Craig Markwardt

>

- > Thanks Craig,
- > your tip was very useful. I never thought about the ERF!
- > Here is the function I am now using:

. . .

- > So far it worked fine!
- > Thanks again.
- > I will see what I can do with the Parinfo parameters. I'm currently using the procedure to show live fitting whilst moving a cross section on an image and it seems stable enough... Fits edges also where one would not see one.

I'm glad that it's working. The reason I suggested PARINFO is that the fitter can get stuck. If it tries to make the step too narrow (P[2] -> 0) during its iterations, then it will have a hard time getting out of that condition in later iterations. A step function with width 0.0001x(grid spacing) gives essentially the same chi-square as a step function with 0.00010001x(grid spacing), so the partial derivative goes to zero, or is noisy.

By setting up PARINFO.STEP, you can make sure that MPFIT takes large enough steps for partial derivatives.

Craig