
Subject: MPFIT

Posted by [Wout De Nolf](#) on Wed, 05 Nov 2008 16:17:07 GMT

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Hi all

Hi Craig ;-)

Every once in a while, when using mpfit with box constraints on some of the parameters, I run into the same problem: I get X+F convergence while the model clearly doesn't fit well to the data.

Today it happened again. I noticed that the last alpha (fraction of the LM-step) equals to 1.4e-017 which makes the actual and predicted reduction of the Chi-Square very small, causing the X and F convergence criteria to be fulfilled.

If alpha is so small, this means that a parameter got close to the boarder in a previous iteration (in my case 1.1e-016, while the lower boarder = 0). When it gets that close, it should have been picked up by this piece:

```
---begin snip mpfit.pro---
```

```
;; Adjust the final output values. If the step put us exactly
```

```
;; on a boundary, make sure it is exact.
```

```
sgnu = (ulim GE 0)*2d - 1d
```

```
sgnl = (llim GE 0)*2d - 1d
```

```
wh = where(qlim AND wa2 GE ulim*(1-sgnu*MACHEP0), ct)
```

```
if ct GT 0 then wa2[wh] = ulim[wh]
```

```
wh = where(qlim AND wa2 LE llim*(1+sgnl*MACHEP0), ct)
```

```
if ct GT 0 then wa2[wh] = llim[wh]
```

```
---end snip mpfit.pro---
```

But it didn't because llim is zero in my case. Am I right in saying that this needs fixing (llim + or - something instead of multiplication)?

Additionally, how small can alpha be before causing actred and prered to be less than FTOL and causing false convergence? When determining alpha, one could then limit it to this smallest value and all steps that cause parameters to go outside their box would be put on the boarder in the code-snip above.

Wout

Subject: Re: MPFIT

Posted by [Craig Markwardt](#) on Sat, 08 Nov 2008 17:36:13 GMT

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On Nov 5, 11:17 am, Wox <s...@nomail.com> wrote:

> Hi all

> Hi Craig ;-)

>

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> of the parameters, I run into the same problem: I get X+F convergence
> while the model clearly doesn't fit well to the data.

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> the LM-step) equals to 1.4e-017 which makes the actual and predicted
> reduction of the Chi-Square very small, causing the X and F
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> boarder in a previous iteration (in my case 1.1e-016, while the lower
> boarder = 0). When it gets that close, it should have been picked up
> by this piece:

...

>

> But it didn't because llim is zero in my case. Am I right in saying
> that this needs fixing (llim + or - something instead of
> multiplication)?

You're right, this is a bug. I posted my probable fix on my website.

> Additionally, how small can alpha be before causing actred and prered
> to be less than FTOL and causing false convergence? When determining
> alpha, one could then limit it to this smallest value and all steps
> that cause parameters to go outside their box would be put on the
> boarder in the code-snip above.

In principal since both values are scaled by ALPHA, this should not be
an issue.

Craig

See my website,

<http://cow.physics.wisc.edu/~craigm/idl/idl.html>
listed under "Curve Fitting"
