
Subject: Another MPFIT question

Posted by [MichaelT](#) on Sat, 11 Oct 2008 21:35:18 GMT

[View Forum Message](#) <> [Reply to Message](#)

Today I discovered MPFIT and I am so excited how well it works (many thanks Craig!).

I ran into one problem, however, which I was not able to solve. Maybe, there is a simple solution.

Among all the parameters I have four whose sum must not be larger than a certain value:

$$0 < c1+c2+c3+c4 < 1.$$

All four parameters may vary between zero and one which I implemented using .limits and .limited. But, how do I implement the additional constraint? Any ideas? It may be too obvious for me to see...

Thanks, Michael

Subject: Re: Another MPFIT question

Posted by [Craig Markwardt](#) on Mon, 13 Oct 2008 10:06:07 GMT

[View Forum Message](#) <> [Reply to Message](#)

MichaelT <michael.theusner@gmail.com> writes:

> Today I discovered MPFIT and I am so excited how well it works (many
> thanks Craig!).
>
> I ran into one problem, however, which I was not able to solve. Maybe,
> there is a simple solution.
> Among all the parameters I have four whose sum must not be larger than
> a certain value:
>
> $0 < c1+c2+c3+c4 < 1.$
>
> All four parameters may vary between zero and one which I implemented
> using .limits and .limited. But, how do I implement the additional
> constraint? Any ideas? It may be too obvious for me to see...

The short answer is that MPFIT does not handle complex inequality constraints, only simple box boundary constraints on each parameter. Vince's suggestion of re-expressing with different parameters is a good one, but as you discovered, all the constraints become difficult.

You may be able to cheat. You could append a special data point which contributes "badness" whenever the parameters go outside of their

desired bounds. For example, if you have 100 data points, you would append a 101st residual, computed something like this,

```
big = 100          ; Bigger than your biggest residual
cc = c1+c2+c3+c4   ; Total
cclimits = [0d, 1d] ; Limits on total
toler = 0.001d     ; Tolerance on limits
yy = (1-tanh((cc-cclimits(0))/toler))/2 + (1+tanh((cc-cclimits(1))/toler))/2

resid[101] = big*yy
```

Since MPFIT simply tries to minimize residuals, the presence of one more residual will be handled just fine. As long as the parameters are within constraints, the 101st residual contributes nothing, but if they begin to touch the constraint, resid[101] will start to grow, and hopefully repel the fitter from going that direction. All untested of course.

The TANH() functions make an inverse box-car shape, but with smooth edges. The smoothness is key, otherwise the fitter will rightly fail due to discontinuities.

Craig

--

Craig B. Markwardt, Ph.D. EMAIL: cbmarkwardt@usenet@gmail.com

Subject: Re: Another MPFIT question
Posted by [MichaelT](#) on Tue, 14 Oct 2008 09:26:42 GMT
[View Forum Message](#) <> [Reply to Message](#)

> You may be able to cheat. You could append a special data point which
> contributes "badness" whenever the parameters go outside of their
> desired bounds. For example, if you have 100 data points, you would
> append a 101st residual, computed something like this,

Thanks, Craig! I'll try it out tonight and report back how well it worked in my case.

Mchael

Subject: Re: Another MPFIT question
Posted by [MichaelT](#) on Tue, 14 Oct 2008 20:00:39 GMT

[View Forum Message](#) <> [Reply to Message](#)

Hi again, I just tried it and it works perfectly! Thanks again!

Michel

Subject: Re: Another MPFIT question
Posted by [Craig Markwardt](#) on Wed, 15 Oct 2008 11:22:32 GMT
[View Forum Message](#) <> [Reply to Message](#)

MichaelT <michael.theusner@gmail.com> writes:
> Hi again, I just tried it and it works perfectly! Thanks again!

Huh. That actually blows my mind. I've never tried that before!

Craig

--

Craig B. Markwardt, Ph.D. EMAIL: cbmarkwardt+usenet@gmail.com

Subject: Re: Another MPFIT question
Posted by [jgrimmond](#) on Thu, 06 Nov 2008 22:03:10 GMT
[View Forum Message](#) <> [Reply to Message](#)

On 15 Oct 2008 07:22:32 -0400, Craig Markwardt
<craigmnet@REMOVEcow.physics.wisc.edu> wrote:

Craig,

> MichaelT <michael.theusner@gmail.com> writes:
>> Hi again, I just tried it and it works perfectly! Thanks again!
>
> Huh. That actually blows my mind. I've never tried that before!
>
> Craig

You are mimicking the penalty function approach to
constraints! (Unless, I am really missing something
here).

jg

Subject: Re: Another MPFIT question

Posted by [Craig Markwardt](#) on Sat, 08 Nov 2008 16:23:44 GMT

[View Forum Message](#) <> [Reply to Message](#)

On Nov 6, 5:03 pm, jgrimm...@yahoo.com wrote:

> On 15 Oct 2008 07:22:32 -0400, Craig Markwardt

>

> <craigm...@REMOVEcow.physics.wisc.edu> wrote:

>

> Craig,

>

>> MichaelT <michael.theus...@googlemail.com> writes:

>>> Hi again, I just tried it and it works perfectly! Thanks again!

>

>> Huh. That actually blows my mind. I've never tried that before!

>

>> Craig

>

> You are mimicking the penalty function approach to

> constraints! (Unless, I am really missing something

> here).

Right, I understand that. The mind-blowing part was that it worked on the first try :-)
