
Subject: Re: Another MPFIT question

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

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MichaelT <michael.theusner@googlemail.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

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