
Subject: Re: constraining parameters in multi-Gaussian 1D fitting
Posted by [Craig Markwardt](#) on Mon, 05 Sep 2005 17:07:42 GMT
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"Jess" <jobrien@mso.anu.edu.au> writes:

- > One constraint I am unable yet to do is: I = would like to be able to
- > tie the peak flux of the Gaussians such that the peak flux of last
- > Gaussian is always greater than that of the first Gaussian.
- > I tried using
- > `parinfo((n_gauss-1)*3).tied = 'GT P[0]'`
- >
- > However the tied structure of parinfo doesn't seem to be meant to
- > accept operators like GT,LT, etc. ...

True. MPFIT's TIED fields are limited to equality constraints only.

...

- > However this requires assigning rather tight bounds to P[0] which I
- > really don't know well. Is there a smarter way I can do this using
- > 'tied' or another structure in parinfo?

One approach is to fit one gaussian at a time starting with the strongest one and working your way down to the fainter ones. This assumes that the peaks are well enough separated that they can be fit in succession. If the peaks are blended, well, that's a tough situation.

Long ago I had somebody trying to do something similar, i.e. fit an arbitrary number of gaussians with arbitrary centroids, widths and amplitudes. I warned him that I thought it would turn into an unconstrained mess, it did, and I think he eventually gave up. Sorry, but least squares fitting is not mind reading. The more external constraints you can apply, based on knowledge of the problem, the better.

Craig

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Craig B. Markwardt, Ph.D. EMAIL: craigmnet@REMOVEcow.physics.wisc.edu
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Subject: Re: constraining parameters in multi-Gaussian 1D fitting

Hi Craig (and everyone else),

Thanks for clarifying the use of "tied". In that case I will have to use limits. Perhaps I can re-fit a velocity profile altering my parinfo limits, if the first multi-Gaussian fit of that profile doesn't yield the right relationship between the peak fluxes of each Gaussian.

Unfortunately I can't sequentially fit single Gaussians, as the velocity profile is a sum of overlapping Gaussians. Each profile comprises emission from a line-of-sight through an edge-on galaxy disk in cylindrical rotation $V(R)$, with gas distribution assumed to be azimuthally symmetric, monotonically decreasing radial flux profile, isothermal and with isotropic velocity dispersion.

Thus I assume to know the following constraints:

- number of gaussians in any profile
- "good" parameter estimates of all but one gaussian in any profile.
- The centroid of the unknown gaussian must be higher than all the others.
- The peak flux of the unknown gaussian should be equal or higher than all the others.
- For the other Gaussians in a profile, each comprising flux from a radial bin higher than R at the line of nodes, the parameters held fixed or strongly limited from having already fitted flux at those radii when analysing velocity profile of sightlines further out. I start at the outermost sightline, where I am only fitting gas at R_{\max} , then fit the next innermost using the kinematics at the higher R sightline as parameter estimates.
- In practice, the centroids of higher R gaussians can be projected to the new sightline and held fixed as they are found accurately in the outer sightline, while the peak flux and velocity dispersion are vulnerable to noise and biased by the telescope spatial beam at the outermost sightlines, so must be bounded for the multi-gaussian fit of the next few sightlines, until they stabilise.

I will try to generate reasonable bounding limits to supply for these high R gaussians, such that the output obeys reasonable assumptions of the input galaxy:

- that radial flux profile is flat or decreasing,
- the centroids of the gaussians at lower radii in line-of-sight profile is always higher than the Gaussian centroids from gas at higher radii projected onto the line of sight.

If this works I should find that the 3 parameter fits of higher radius Gaussian gas components in a sightline profile should stabilise after a few sightline profiles, as I fit that gas component in successive

sightlines. Thus the multi-gaussian fit to each profile should have few unknowns, 3 due to the unknown gaussian at the line-of-nodes radius, the dispersion and peak flux of the next couple of gaussians, say 3-4. So I never have more than 8-11 unknowns, though less in the outermost profiles with fewer gaussians. One advantage of an exponential decreasing radial flux profile is that the poor fits to the highest r components, while they affect the velocity profile fit of the next innermost sightline, they become unimportant, providing its fitting the line-of-node gaussian well.

What do you think Craig? Is the solution too degenerate to be solved with curvefit algorithms like mpfit, despite the heavy constraints I am trying to place on most of the parameters in the multi-gaussian curve fit?

Thanks for your advice,
Jess

Subject: Re: constraining parameters in multi-Gaussian 1D fitting
Posted by [JD Smith](#) on Tue, 06 Sep 2005 00:33:31 GMT
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On Mon, 05 Sep 2005 12:07:42 -0500, Craig Markwardt wrote:

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>
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What if you availed yourself of the ITERPROC procedure to enforce the constraint, dragging the fitter (kicking and screaming if necessary) back into line if it attempts to step out? Any reason this wouldn't work?

JD

Subject: Re: constraining parameters in multi-Gaussian 1D fitting

Posted by [Craig Markwardt](#) on Tue, 06 Sep 2005 01:58:54 GMT

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"Jess" <jobrien@mso.anu.edu.au> writes:

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> in cylindrical rotation $V(R)$, with gas distribution assumed to be
> azimuthally symmetric, monotonically decreasing radial flux profile,
> isothermal and with isotropic velocity dispersion.
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... extensive description deleted ...
>
> What do you think Craig? Is the solution too degenerate to be solved
> with curvefit algorithms like mpfit, despite the heavy constraints I am
> trying to place on most of the parameters in the multi-gaussian curve
> fit?

Sorry, I got a bit lost in that description.

If possible, I would try to fit the "new" peak while holding the other peaks absolutely constant, and then only after the "new" peak fit has converged, allow more of the parameters to vary. You want to be as close as possible to the optimal solution before you allow the most parameters to vary.

Happy fitting,
Craig

--

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Subject: Re: constraining parameters in multi-Gaussian 1D fitting

Posted by [Craig Markwardt](#) on Tue, 06 Sep 2005 02:35:15 GMT

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JD Smith <jdsmith@as.arizona.edu> writes:

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```

It might work, it might not. I suspect that in general the fitter might get stuck. For example, if we *started* out by thinking the tallest peak was on the left part of the curve - and made a model function to match that - but the truth is that a peak on the right is truly the tallest, then we can enforce all the constraints in the world and won't come out with the best fit.

Now, with the additional info that the original poster provided, this will probably not be the case, so s/he might be alright.

Craig

--

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