
Subject: Re: find missing elements in an array

Posted by [Helder Marchetto](#) on Wed, 09 Jan 2013 22:44:48 GMT

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On Wednesday, January 9, 2013 11:08:55 PM UTC+1, Craig Markwardt wrote:

> On Wednesday, January 9, 2013 3:56:47 PM UTC-5, Brian Cherinka wrote:

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>> On Monday, January 7, 2013 3:02:22 PM UTC-5, Craig Markwardt wrote:

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>>> On Monday, January 7, 2013 10:37:44 AM UTC-5, Brian Cherinka wrote:

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>>>> On Thursday, December 27, 2012 1:37:48 PM UTC-5, Brian Cherinka wrote:

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>>>> > I have a peak-finding routine that finds, well...peaks, in a larger array. I know how many peaks there are suppose to be, and I know the way they should be arranged, e.g.

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>>>> > 1 set of 5 peaks, a gap, then a set of 10 peaks, a gap, then a set of 7 peaks etc....
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>>>> > and I know how many sets of peaks there are as well. But sometimes these peaks could
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and the expected values.
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>>>> > so with the above example, I know there should be 22 peaks total in an array of data of
say 30 elements, grouped in 3 sets of [5,10,7] peaks. I don't know where the peaks are apriori in
the large array of 30 elements or where they should be.
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>>>> > If I find 20 peaks, I know there are 2 missing but I would like to find out which peaks they
are, in what sets, and where in the data array of 30 elements they are. Any ideas?
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>>>> > I have a current method in place involving using the separations between found peaks
but it is bulky, and inconsistent. I am looking for alternative methods or help in making the method
I do have implemented more efficient. Below I will describe my currently attempted method.
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>>>> > If all peaks were found then the separations (element+1 - element) should be something
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>>>> > seps = [5,4,5,6,15,11,10,11,12,12,12,11,11,10,14,4,4,5,6,4,5,4] 22 elements
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>>>> > and I know there should be 2 gaps that separate the 3 bundles ; the 15 and the 14
indicate gap locations.
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>>>> > seps = [5,4,5,6,15,11,10,11,16,12,11,11,10,12,4,4,10,4,5,4] 20 elements ; here a
missing peak is in the 2nd and 3rd sets.
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>>>> > I do have an array of expected separation between peaks in the sets, so [5,11,4] would
be the expected (or lets say median) separations in the above example. So I basically loop over
each set and look for regions in the seps array where the value is greater than the expected
value; basically looking for the gaps. If all the peaks are there I only find 2 gaps. In the above
example of 2 missing peaks, I find 4 gaps and can figure out that there are 2 missing peaks and
where they are and in which sets. I've had to refine it (and make it more complicated) where the
separation decreases from 1 set to the next, as in the above set 2 to set 3 transition. But it's still
inconsistent. It mostly works but if the separation values are different by 1 or 2, then my code isn't
very robust. The problems come in then with using equalities (LE,GE) vs not (LT,GT) and the fact
the the actual separations can vary up or down from the expected value.
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>>>> > My loop here is something like this, with, for the above example, nbundle=3,
medsep=[5,11,4] is the expected separation, ntot = [5,15,22] is the cumulative total of the number
of peaks in each set =[5,10,7]
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>>>> > tmp=where(seps gt medsep[0]+2)
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>>>> > test=[test,tmp[where(tmp lt ntot[0])]]
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>>>> > nt=n_elements(test)
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>>>> > if bid eq 1 then begin
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>>>> > ;refinement to handle the set 2 to 3 transition with the decrease which I've had to
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>>>> > tmp=where(sep[test[nt-1]+1:n_elements(sep)-1] le medsep[bid+1])+test[nt-1]+1
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>>>> > tmp = tmp[where(tmp+(indgen(n_elements(tmp))) le ntot[bid]+1)]-2
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>>>> >   if n_elements(tmp) gt 1 then tmp=tmp[n_elements(tmp)-1] ; in place in case it finds a
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>>>> >   test=[test,tmp]
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>>>> >      tmp=where(sep[test[nt-1]+1:n_elements(sep)-1] ge medsep[bid]+2)+test[nt-1]+1
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>>>> >      test=[test,tmp[where(tmp+(indgen(n_elements(tmp))+1) le ntot[bid])]]
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>>>> > gaps = test[where(test gt 0)]
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>>>> > It actually gets more complicated than this because I first look for missing peaks within
sets, and then I look for missing peaks at the edges of sets which involves very similar code, well
the same code to find gaps, and then different code to ascertain whether it's a missing edge or
not. If I could simplify these two stages down into one, that would be great as well.
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>>>> > I'm looking for something that will be robust because this needs to be automated and be
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>>>> > I think this about covers it. :)
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>>>> > Can value_locate solve my problem? Any help would be appreciated. Thanks. :)
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>>>> Does anyone have some thoughts on this? I could use some help on this problem. This is
becoming quite buggy and finicky and I've already added too many bandaids.
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>>> I wondered if you could try a cross-correlation technique. You know where your peaks
should be, so you can create a template mask. You can slide this template across your data to
find matches, a la C_CORRELATE(). A missing peak wouldn't contribute to the correlation
amplitude, but it shouldn't subtract either. I don't know how bar-code readers work, but I suspect
it is this way.
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>>> Best wishes,
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>>> Craig
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>> Well I don't actually know beforehand where the peaks are supposed to be. I just know how
many peaks there should be and how they are arranged (in so many groups of so many peaks
with this expected spacing). My first step is to find the supposed peaks and their locations then I
do this complicated business of looking for peaks missing if it doesn't find how many it's suppose
to. I guess I could build a model based off the first pass of finding supposed peaks.
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> I don't get it. What are the knowns and unknowns?
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> I had assumed that you knew the *relative* positions of the peaks, but the absolute position is
unknown. That is, aside from a single global positional offset, you know what the spectrum should
look like ahead of time.
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> If that's the case, you can make a template spectrum with the correct spacing of the peaks.
Cross correlation allows you to slide the template across your measured spectrum until you get a
match. Missing peaks are OK, since they simply do not add to the correlation amplitude, but the
peaks that are present do add.
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>
> You mentioned something about groups. I don't know what that means. If it means that each group has its own offset, that's OK: in principle you can make different templates for each group, and slide them one at a time.
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> Doing it the way you are doing it, you need to account for *all* possible combinations of missing peaks, which is a huge number. Good luck.
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> Craig

I think Craig's suggestion is the only way to go. If I understand your problem correctly, and I think Craig already made the point, you have spectra (I'm guessing something like rotational or vibrational molecular spectra) that you want to find. If you know what molecules you expect having groups of peaks with characteristic distances, by constructing these spectra artificially, you can do a cross-correlation of the data and the artificial data. Just in case you're not sure about this, look at the picture in wiki:

http://en.wikipedia.org/wiki/File:Convolution_of_box_signal_with_itself2.gif

It's well done. When the data and model peaks overlap, you get a maximum in the cross-correlation.

I hope it helps...
cheers,
Helder
