Subject: speed, size, contouring
Posted by Hawaiianite on Thu, 02 Aug 2007 00:44:00 GMT
View Forum Message <> Reply to Message

Hello all,

Curious if you have some suggestions about a program I'm trying to run. Basic scenerio is I have a large array (176851) of mineralogy (4 minerals) and their model spectra. I take one of them replicate it to the size of the original array and then compare it to all of them at once. I take the ones that are within a criteria I call excursion (band with max difference between original spectrum and another model spectrum) and then I see how close their mineralogy is to that spectrum of interest. I want to do that for each composition/spectrum I'm looking at and make a contour diagram of my results for each mineral.

There are three areas in which I am struggling. Speed, size, and the contouring feature. It takes about 190 seconds just to do 100 model compositions (for some reason I've struggled to get around for loops in this case). In regards to size some spectra often have many close matches especially if I'm only trying to match 4 bands rather than eight of the spectrum. I've found once I get about 65 matches the array becomes too large for my computer to handle. I'm also struggling with the putting the results into a contoured ternary diagram (this I have done before, but with different data a long time ago). For this I keep getting the error "CONTOUR: Contour levels must be in increasing order." I've just never gotten this error before and I'm having a little trouble deciding what it is referring to.

thanks,
Hawaiianite

```
pro minexcur,bands,n,m
 ;=============================================================
====================
;WAVES--THE WAVELENGTHS CHOSEN TO BE MODELED (NEEDS TO BE DEFINED
BELOW)
   waves=[0.75, 0.90, 0.95, 1.0,1.1, 1.25, 1.50, 2.0]
   numwaves=(size(waves))(1)
   ;BANDS--NUMBER OF BANDS IN SPECTRUM WILL BE COMPARING
   ;N--REFERS TO A NUMBER OF MODELS TO COMPARE (TO GET PROGRAM UP AND
RUNNING AND THEN INCREASE SPEED)
   ;M--REFERS TO THE MINERAL YOU WILL BE USING
   ;MG--THE SPECIFIC MG-NUMBER ENTERED FOR THIS MODEL(NEEDS TO BE
DEFINED BELOW)
   ;VEC--IS A 12 ELEMENT VECTOR OF MINERALOGY AND CHEMISTRY.
t1=systime(1)
```

```
 ;=============================================================
====================
;READ IN MODEL SPECTRA
 ;=============================================================
====================
vec=12.
index=176851.
nummat=1.
mgs=1                                                ;HOW
MANY MG' MODELS TO LOAD
mginc=20                                              ;MG'
INCREMENT TO LOAD
mod_out=fltarr(vec+numwaves,nummat*index,mgs)   ;OUT_VEC+ABS.
REFLECTANCE

for i=0,mgs-1 do begin
    vecspec=fltarr(vec+numwaves,index*nummat)
     filename2=string('outvs_min_07112007_',strtrim(55+i*mginc,2) )
    openr,2,filename2,get_lun
    readu,2,vecspec
    mod_out[*,*,i]=vecspec[*,*]
    close,/all
endfor
t2=systime(1)
print,systime(1)-t1,' Seconds'
 ;=============================================================
====================

 ;=============================================================
====================
;CALCULATIONS
 ;=============================================================
====================
excur=fltarr(nummat*index)
a=fltarr(bands)
out_arr=fltarr(21,nummat*index,65)
av_arr=fltarr(1,nummat*index)
for j=0L,n-1 do begin
 a[*]=mod_out[12:bands+11,j]
 a[*]=a[*]/mean(a)
 reparr=rebin(a,bands,nummat*index)
 for i=0L,nummat*index-1 do begin
    mod_out[12:bands+11,i]=mod_out[12:bands+11,i]/mean(mod_out[1 2:bands
+11,i])
         excur[i]=max(abs(mod_out[12:bands+11,i]-
reparr[0:bands-1,i]))
 endfor
```

```
 d=where(excur gt .005 and excur lt .00501)

 s=(size(d))(0)
 p=(size(d))(1)
 print,string('Model#= ',strtrim(j,2),' Min=  ',strtrim(mod_out[0:3,j],
2),' # of matches = ',strtrim(p,2))
 if (s gt 0) then begin
  out_arr[0:19,j,0:p-1]=mod_out[*,d[*]]
  out_arr[20,j,0:p-1]=excur[d[*]]
  modminrep=mod_out[0:3,j]
  modminrep=rebin(modminrep,4,p)
  matches=fltarr(4,p)
  for k=0,p-1 do matches[*,k]=out_arr[0:3,j,k]
  mindif=fltarr(4,p)
  for k=0,p-1 do mindif[*,k]=abs(modminrep[*,k]-matches[0:3,k])
  av_arr[*,j]=mean(mindif[m,0:p-1])
 endif
endfor
t3=systime(1)
print,systime(1)-t2,' Seconds'
 ;=============================================================
==================

 ;=============================================================
==================
;TRIANGULATE THE DATA POINTS FOR CONTOUR PROCEDURE.
 ;=============================================================
==================
    x=(mod_out[2,0:n-1]+mod_out[3,0:n-1])*100
    y=(mod_out[3,0:n-1]*(sqrt(3)/2))*100
    z=av_arr[*,0:n-1]*100

    window,2,xsize=640,ysize=640
    contour,z,x,y,LEVELS=fix(findgen(15) * ((max(z) - min(z))/15) +
min(z)) ,$
     background=255,c_color=0,c_linestyle=2,c_labels=fix(findgen( 15) *
((max(z) - min(z))/15) + min(z)),$
    c_charsize=1.5,ymargin=7,xmargin=7,c_thick=1,/irregular
    image=tvrd()
    contour,z,x,y,/fill,LEVELS=fix(findgen(15) * ((max(z) - min(z))/
15) + min(z)) ,$
    background=255,c_labels=fix(findgen(15) * ((max(z) - min(z))/15) +
min(z)),c_charsize=1.25,ymargin=7,xmargin=7;,/irregular
    image2=tvrd()
    tvscl,image/2+image2/2

    ;DEFINE OUTLINE OF THE TERNARY.
    ;Define bottom of triangle.
```

```
   x1=findgen (101.0)
   y1=fltarr(101.0)
   oplot, x1,y1, color=0,thick=2

   ;Define OPX to Pl side of triangle.
   x2=findgen(51.0)
   y2=1.732*x2
   oplot, x2,y2, color=0,thick=2

   ;Define CPX to Pl side of triangle
   x3=findgen (101.0)
   y3=-1.732*x3+173.2
   oplot, x3[50:100],y3[50:100], color =0,thick=2
   ;oplot, x,y,psym=5, color=0

   ;Define Rock Type Regions.
   y4=fltarr(101.0)+77.9
   oplot, x3[45:55],y4, color=0, thick=1,linestyle=0
   y5=fltarr(101.0)+67.1
   oplot, x3[39:61],y5, color=0, thick=1,linestyle=0
   y6=fltarr(101.0)+52
   oplot, x3[30:70],y6, color=0, thick=1,linestyle=0
   y7=fltarr(101.0)+8.7
   oplot, x3[5:95],y7, color=0, thick=1,linestyle=0
   y8=findgen(101.0)
   x4=fltarr(101.0)+50
   oplot, x4, y8[9.0:78.0], color=0, thick=1, linestyle=0
   y11=-1.732*x3+155.88
   oplot, x3[60:85],y11[60:85], color =0,thick=1, linestyle=0
   y12=1.732*x3-17.32
   oplot, x3[15:40],y12[15:40], color =0,thick=1, linestyle=0

   AXIS, YAXIS =0, color=255
   AXIS, YAXIS =1,  color=255
   AXIS, XAXIS=0, color=0,charthick=1.5, charsize=1.8
   AXIS, XAXIS=1, color=255
   xyouts, 315, 550, '!8PL', /device, color=0,charsize=3,charthick=2
   xyouts, 40, 10, '!8OPX', /device, color=0,charsize=3,charthick=2
   xyouts, 560, 10, '!8CPX', /device, color=0,charsize=3,charthick=2
 ;=============================================================
==================
stop
end
```