Self modeling curve resolution

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Author has carried out one experiment in spectrophotometry, and has received 5 samples of material from an experimental production process.

Then he plotted the data on the **absorbance Vs. Wavelength graph**.
And he got the five curves as shown in the figure.

Now the first step in the analysis is to whether or not the two dye mix hypothesis is reasonable. And for that he carries out the principle component analysis. He successfully got the two dominating eigen vectors V1 & V2.

Then he calculated the error of fit and he again plotted the original vector with the list square fit and yielded the five graphs shown .

Then he plotted a graph

Seic 1 Vs Seic 2

So as to get the position of the **n11, n12, n21 and n22**

He made all the restriction to get the position of those points .
He then got the two regions called A1 and A2 and the line intersecting these two regions gave the values of **F1*, F2*, F1**, F2**.**

Then he successfully resolved the original curve in to two two distinct curve areas which shows that one band is of dye A and the other one is of Dye B.

The Program to get those graphs and to resolve the curve is given as follows

Language : MATLAB

```
global E1 E2 v1 v2 Matrix j yy n nc F1star F2star ycomp
Matrix=[0.924 2.478 1.239 0.413 2.774;
   4.406 8.006 6.845 5.075 11.920;
   5.488 9.009 10.110 6.393 18.392;
   6.530 11.900 11.586 9.009 20.969;
   4.977 9.422 10.307 7.475 16.681;
   4.898 8.419 8.242 6.452 13.907;
   3.875 6.432 6.845 4.839 10.878;
   3.600 6.157 6.255 4.485 10.032;
   3.501 4.780 5.272 3.796 8.439;
   4.878 5.429 5.724 4.917 7.534;
```

```
    9.992 9.953 9.678 8.950 9.068;
    16.739 16.601 17.762 15.815 12.845;
    27.341 27.715 28.521 26.653 20.083;
    40.146 44.041 42.566 42.015 33.321;
    52.735 62.570 58.085 55.155 48.752;
    54.801 72.995 66.858 62.944 70.262;
    51.260 80.155 70.405 66.701 88.633;
    46.775 81.512 73.448 66.937 98.350;
    39.832 74.962 68.353 60.623 97.800;
    30.272 64.950 57.613 52.676 88.240;
    22.463 51.496 45.969 39.969 72.799;
    15.795 34.875 34.442 30.154 55.352;
    11.350 25.728 25.079 21.303 41.189;
    7.947 17.900 17.703 15.087 30.135;
    4.760 11.271 11.684 9.796 20.103;
    2.813 7.317 7.140 5.842 13.632;
    2.065 4.485 4.544 3.698 8.065;
    1.593 2.813 2.655 2.419 5.134;
    0.964 1.436 1.318 1.259 2.833;
    0.669 0.472 0.079 0.138 0.551];
nr=length(Matrix(:,1))
nc=length(Matrix(1,:))
Mean=mean(Matrix);
%disp('Mean of the matrix  =')
%disp(Mean);
%this loops is to calculate the mean of the matrix
for i=1:nr
    for j=1:nc
        diffmean(i,j)=Matrix(i,1)-Mean(1,j);
    end
end
%disp(diffmean);
trans=diffmean';
Sqmat=diffmean*trans;
%disp(Sqmat);
%this loop is to plot the original data set which  appears in figure one
x=410:10:700;
for j=1:nc
     for i=1:nr
         y(i,j)=Matrix(i,j);
         hold on
     end
     plot(x,y)
     j=j+1;
end
figure
```

```
hold off;
transpose=Matrix';
    Sqmatrix=Matrix*transpose;
    M=Sqmatrix/30;
    [u,M]=eigs(M,2);
    v1=u(:,1)
    v2=-1*u(:,2)
    V1trans=v1';
    A=V1trans*v1;
    disp(A);
    %from here it starts the calculation for seic 1 and 2 by square method
    for j=1:nc
     for i=1:nr
         y(i,j)=Matrix(i,j);
     end
     yy=Matrix'
     for j=1:nc
         seic11=50;
         seic21=50;
         xo=[seic11 seic21];
         options=1;
         xopt=fmins('leastsquare',xo,options)
         seic1opt(j)=xopt(1);
         seic2opt(j)=xopt(2);
     end
     seic1=seic1opt
     seic2=seic2opt
     %from here it starts the calculation for seic 1 and 2 by square method
     seic1comp=v1'*y
     seic2comp=v2'*y
     j=j+1;
end
    disp('seic1 = ')
     disp(seic1)
     disp('seic2 = ')
     disp(seic2)
     %here starts the while loop to calcualte the Y least square
for j=1:5
    for i=1:30
     ycomp(i,j)=v1(i,1)*seic1(1,j)+v2(i,1)*seic2(1,j);
 end
 plot(x,ycomp(:,j),x,y(:,j))
     figure
     axis([400 700 0 100]);grid
  j=j+1;
 end
```

```
 %this loop is to calculate the values of K+
for i=1:30
    if v2(i,1)>0
        K1(i,1)=v1(i,1)/v2(i,1);
    end
end
disp('K1')
disp(K1)
%this loop is to calculate the values of K-
for i=1:30
    if v2(i,1)<0
        K2(i,1)=v1(i,1)/v2(i,1);
    end
end
disp('K2')
disp(K2)
eita=-min(abs(K1));
theta=min(abs(K2));
disp('eita')
disp(eita)
disp('theta')
disp(theta)
for i=1:5
    ratio(1,i)=seic2(1,i)/seic1(1,i);
end
disp('ratio')
disp(ratio)
U=max(ratio)
V=min(ratio)
disp(U)
disp(V)
%calculationg for C1 and C2
C1=sum(v1)*10
C2=sum(v2)*10
%calculation for siec1 for plotting the error function
seicA=1/(C1+eita*C2)
seicB=1/(C1+theta*C2)
seicC=1/(C1+U*C2)
seicD=1/(C1+V*C2)
%calculation for siec2 for plotting the error function
seicA1=eita/(C1+eita*C2)
seicB1=theta/(C1+theta*C2)
seicC1=U/(C1+U*C2)
seicD1=V/(C1+V*C2)
%calculation for F1*, F2*, F1**, and F2**
F1star=seicA*v1+seicA1*v2
```

```
F2star=seicB*v1+seicB1*v2
F1doublestar=seicC*v1+seicC1*v2
F2doublestar=seicD*v1+seicD1*v2
% Calculation for the intersecting line and
%F1lamda=a*F1star+(1-a)*F1doublestar
%F2lamda=b*F2star+(1-b)*F2doublestar;
figure
plot(x,F1star,'b',x,F2star,'g',x,F1doublestar,'g',x,F2doublestar,'b')
figure
hold off
plot(x,F1star,'b',x,F2star,'g')
figure
%From here starts the program for Plot-2
seic1=0:40:240;
YY=1/C2-(C1/C2)*seic1
slope=eita*seic1;
slope1=theta*seic1;
seicm=U*seic1;
seicmi=V*seic1;
xaxis=0*seic1;
plot(seic1,YY,'b',seic1,xaxis,'r',seic1,slope,'g',seic1,slope1,'g',seic1,seicm,'b',seic1,seicmi,
'b',seicA,seicA1,'*',seicB,seicB1,'*',seicC,seicC1,'*',seicD,seicD1,'*')
axis([0 240 -40 40]);grid
figure
%End of plot-2
%here starts the program for the calcualtion of alfa and beta value
for j=1:nc
    for i=1:nr
        y(i,j)=Matrix(i,j);
    end
    yy=Matrix'
    for j=1:nc
        alfa=50;
        beta=50;
        x1=[alfa beta];
        options=1;
        xopt=fmins('alfabeta',xo,options);
        alfaopt(j)=xopt(1);
        betaopt(j)=xopt(2);
    end
    alfa=alfaopt
    beta=betaopt
    j=j+1;
end
%here ends the program for the calcualtion of alfa and beta value
for j=1:5
```

```
    for i=1:30
        Istcurve(i,j)=alfa(1,j)*F1star(i,1);
        seccurve(i,j)=beta(1,j)*F2star(i,1);
        commcurve(i,j)=Istcurve(i,j)+seccurve(i,j);
    end
    plot(x,Istcurve(:,j),'r')
    hold on
    plot(x,seccurve(:,j),'r')
    hold on
    plot(x,commcurve(:,j),'r')
    hold on
    plot(x,y(:,j),'b')
    figure
    j=j+1;
    hold off
end
```

<u>We have written a subroutine program : leastsqaure.m</u>

```
function f=leastsquare(x)
global E1 E2 v1 v2 Matrix j yy n nc F1star F2star ycomp
seic1=x(1);
seic2=x(2);
v1prime=v1';
v2prime=v2';
sumaes=0;
for i=1:30
    ycalculated(i)=seic1*v1prime(i)+seic2*v2prime(i);
    error(i)=yy(j,i)-ycalculated(i);
    err(i)=error(i)^2;
    sumaes=sumaes+err(i);
end
f=sumaes;
```

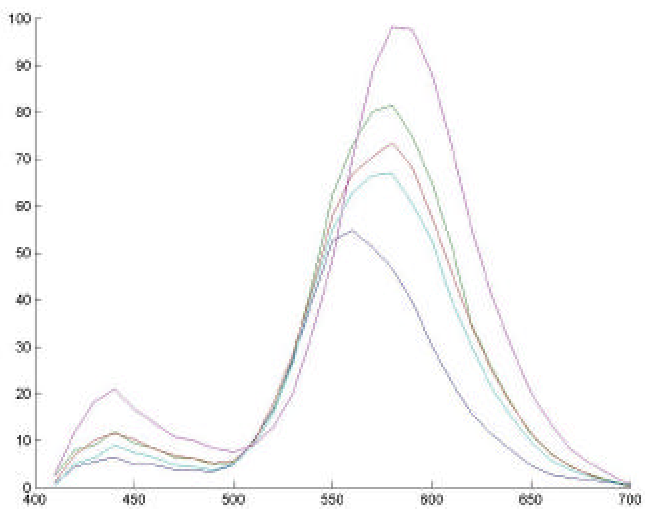
<u>Subroutine : alphabeta.m</u>

```
function f=alfabeta(x)
global E1 E2 v1 v2 Matrix j yy n nc F1star F2star ycomp
alfa=x(1);
beta=x(2);
F1prime=F1star';
F2prime=F2star';
sumaes1=0;
for i=1:30
    ycalculated(i)=alfa*F1prime(i)+beta*F2prime(i);
```

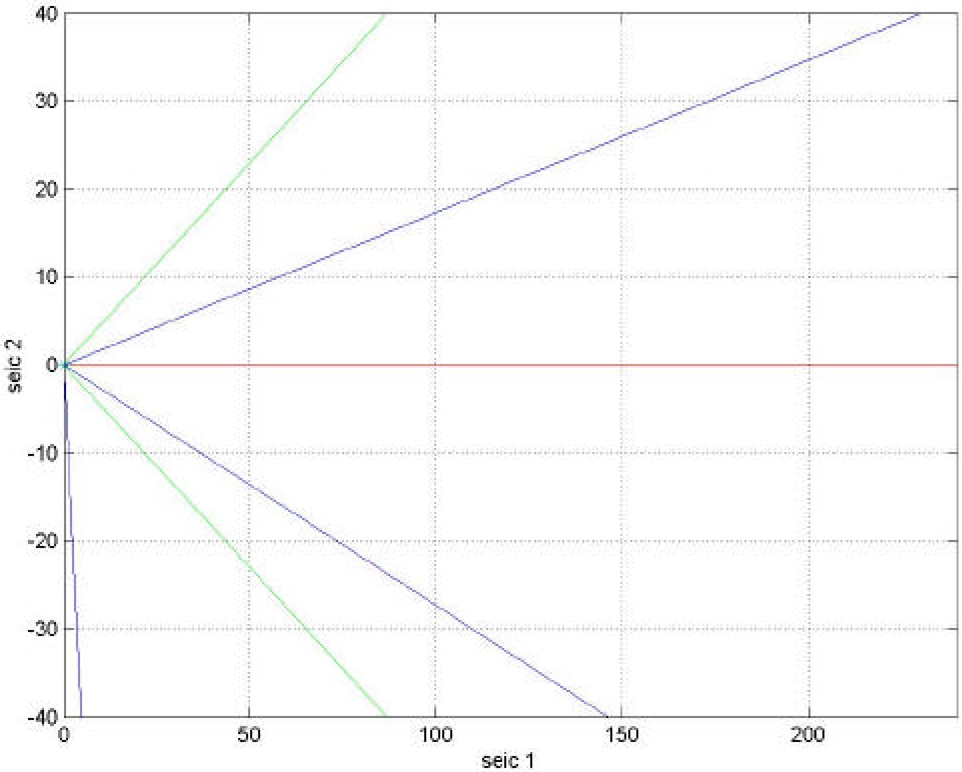
```
   error(i)=yy(j,i)-ycalculated(i);
   err(i)=error(i)^2;
   sumaes1=sumaes1+err(i);
end
f=sumaes1;
```

<u>After running this program we got the following illustrations :</u>

The original data plotted by the author is as follows :

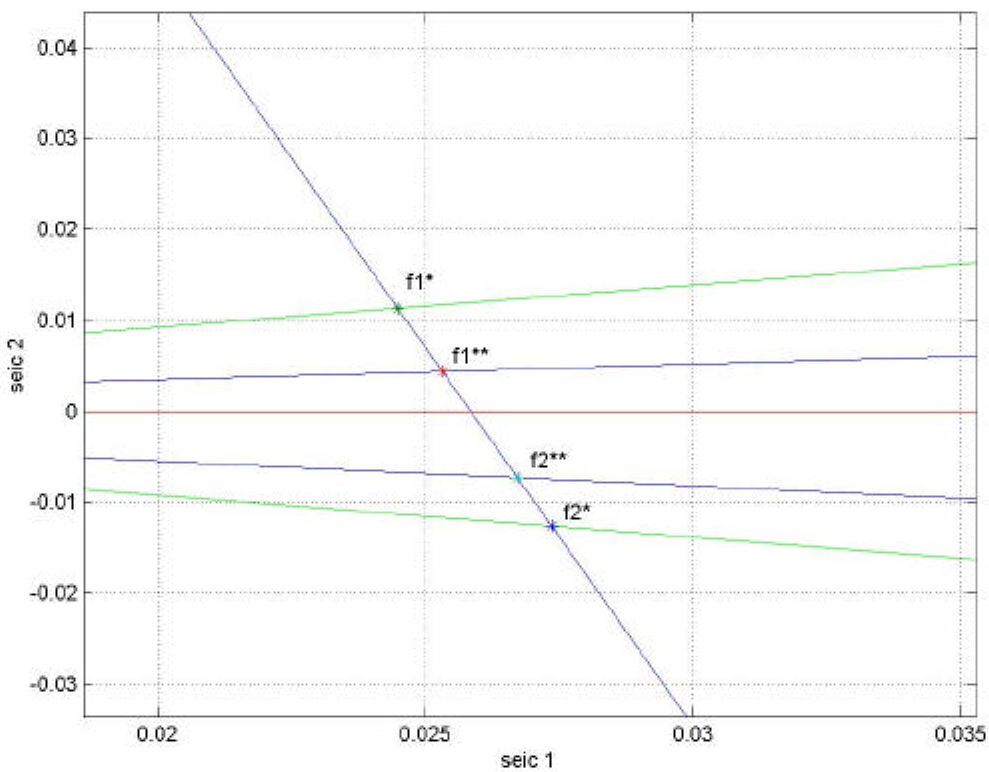


Then we got the seic1 Vs seic2 plot as

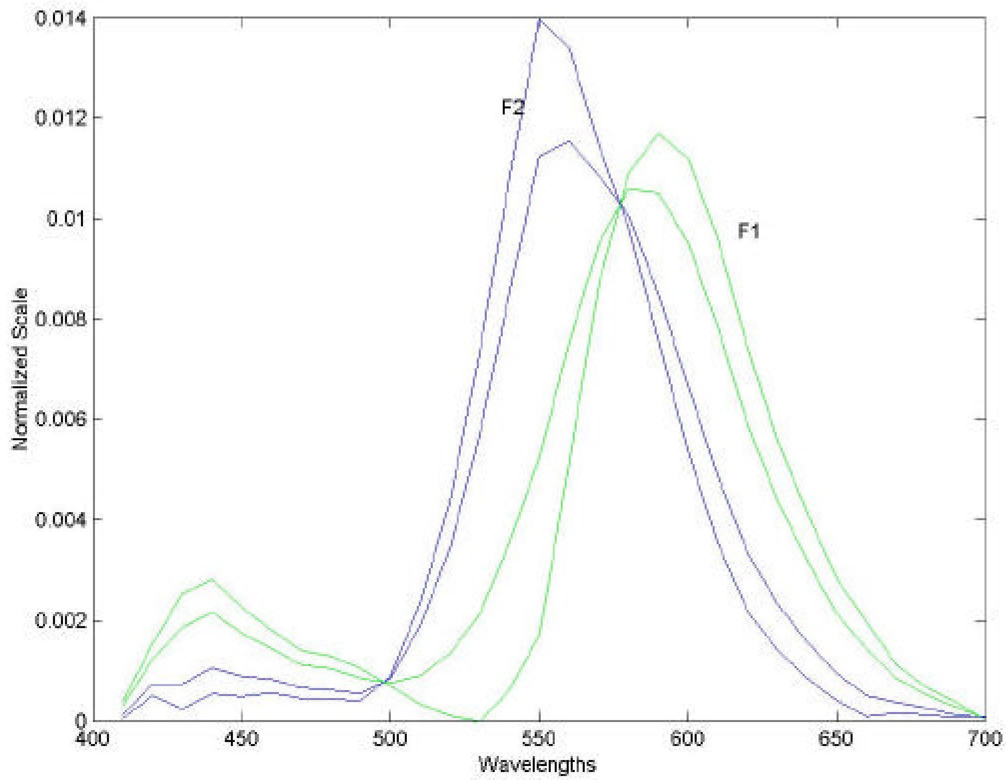


40
30
20
10
0
-10
-20
-30
-40
0
50
100
150
200
seic 1
seic 2

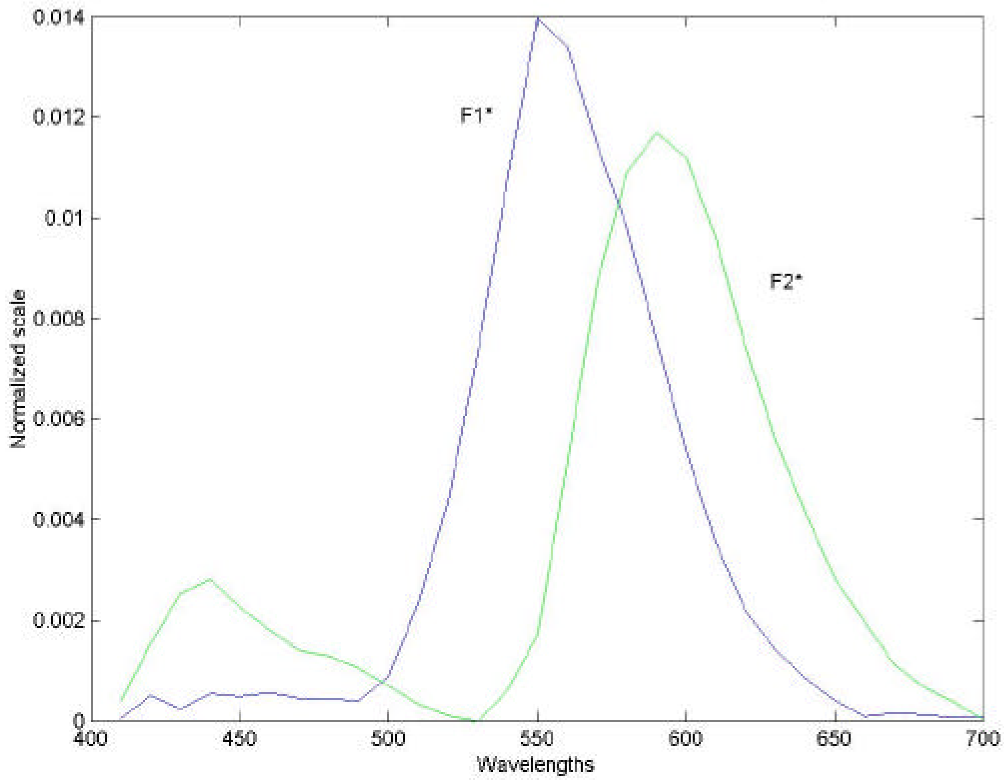
Then expanding the region where line crosses and gives F1*, F1**, F2*, F2** we get



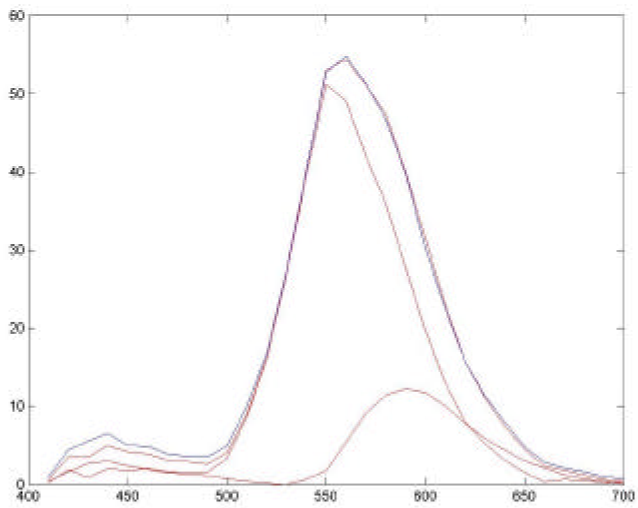
Then we just separated the two regions FI & F2 showing resolved curves we get

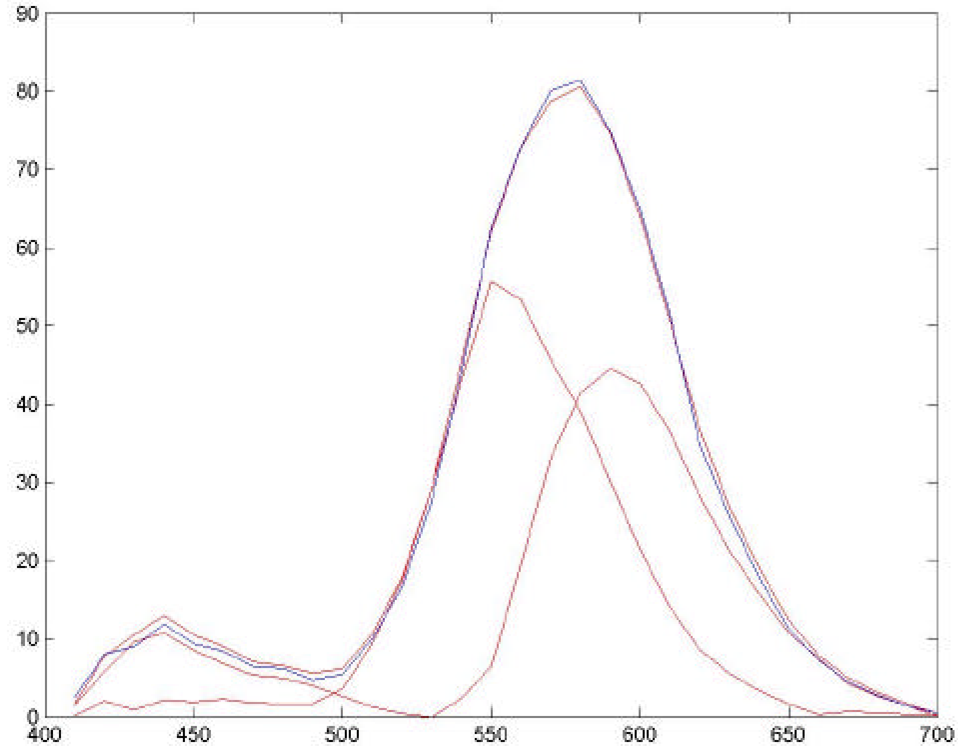


Then we got the final resolvement of the 5 curves in to two main components



Then we have calculated the errors of fit and then plotted original curve , curve with minimum error , and pure components F1 and F2 we got the five graphs as


60
50
40
30
20
10
0
400
450
500
550
600
650
700


90
80
70
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50
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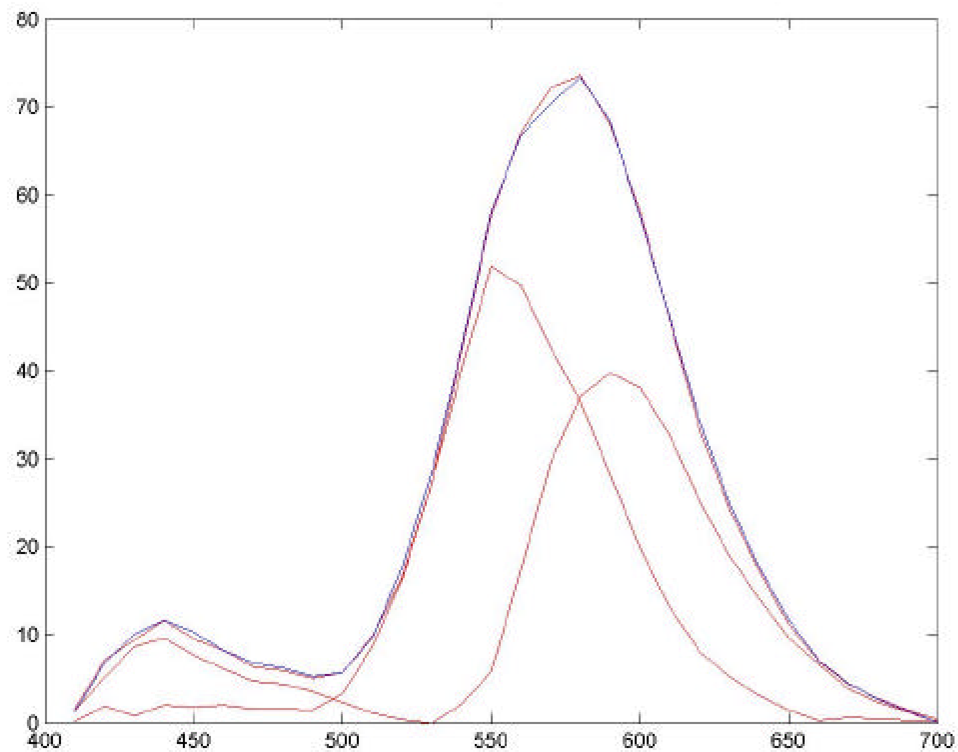
10
0
400
450
500
550
600
650
700


80
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40
30
20
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0
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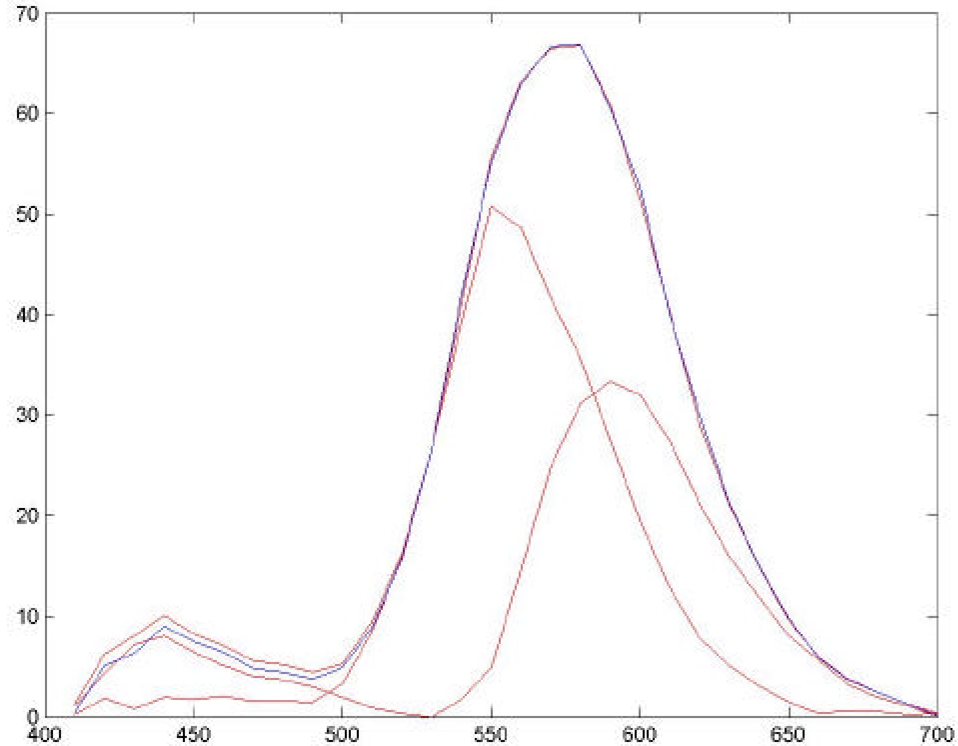
700



70
60
50
40
30
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600
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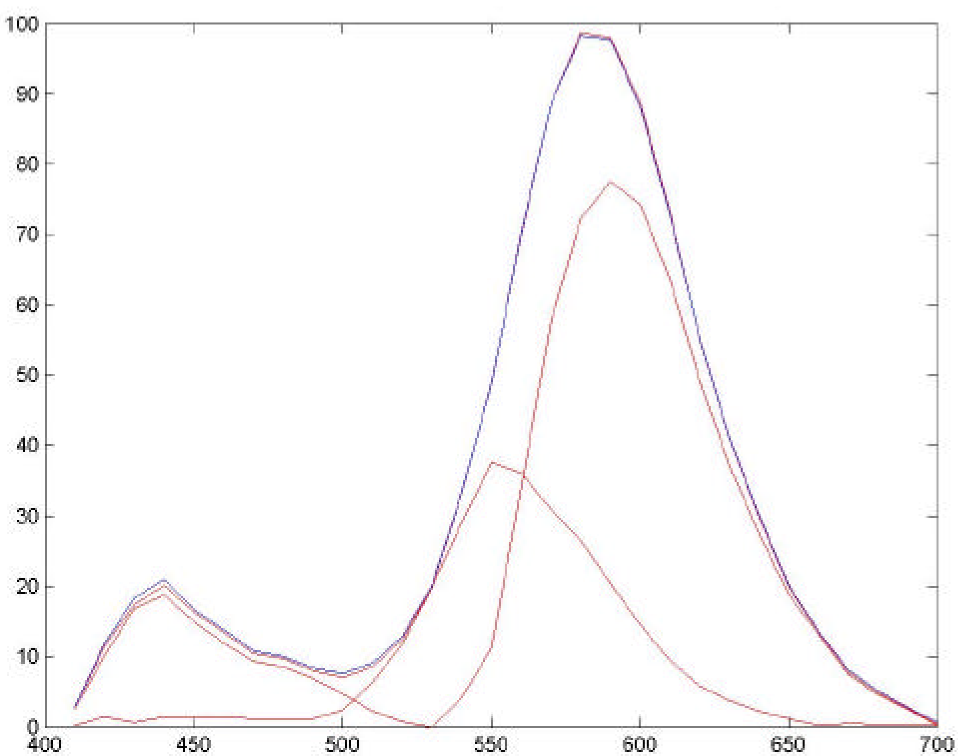
700



100
90
80
70
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40
30
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10
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400
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550
600
650
700