```
% gda01_04
%
% model Mars rover Mossbauer spectra using Lorentzian curves
% supports Figure 1.4

clear all;

% load data
D=load('../data/mars_soil.txt');
v=D(:,1);
d=D(:,2);
d=d/max(d); % normalize
N=length(d);

% delete negative velocities
i=find(v>=0,1);
v=v(i:N);
d=d(i:N);
N=length(v);

% plot data
figure(1);
clf;
set(gca,'LineWidth',3);
set(gca,'FontSize',14);
hold on;
axis( [0, 12, min(d), max(d)] );
plot(v,d,'r-','LineWidth',2);
plot(v,d,'ro','LineWidth',3);
xlabel('velocity, mm/s');
ylabel('counts');
title('click bottom of each peak, then left of axis');

% lorentzian curve of peak amplitude a, center velocity v0 and width c
% f(v)   = a c^2 / ( (v-v0)^2 + c^2) )
% df/da  = c^2 / ( (v-v0)^2 + c^2) )
% df/dv0 = 2 a c^2 (v-v0) / ( (v-v0)^2 + c^2) )^2
% df/dc  = 2 a c / ( (v-v0)^2 + c^2) ) - a c^3 / ( (v-v0)^2 + c^2) )^2
% 3 model parameters per lorentzian, (a, v0, c)

% estimate of backgroind level
A = max(d);

% number of peaks determined by clicking on graph
disp('click on the bottom each peak');
```

```
click on the bottom each peak
```

```
disp('    click to the left of zero when done');
```

```
    click to the left of zero when done
```

```
disp(' ');
```

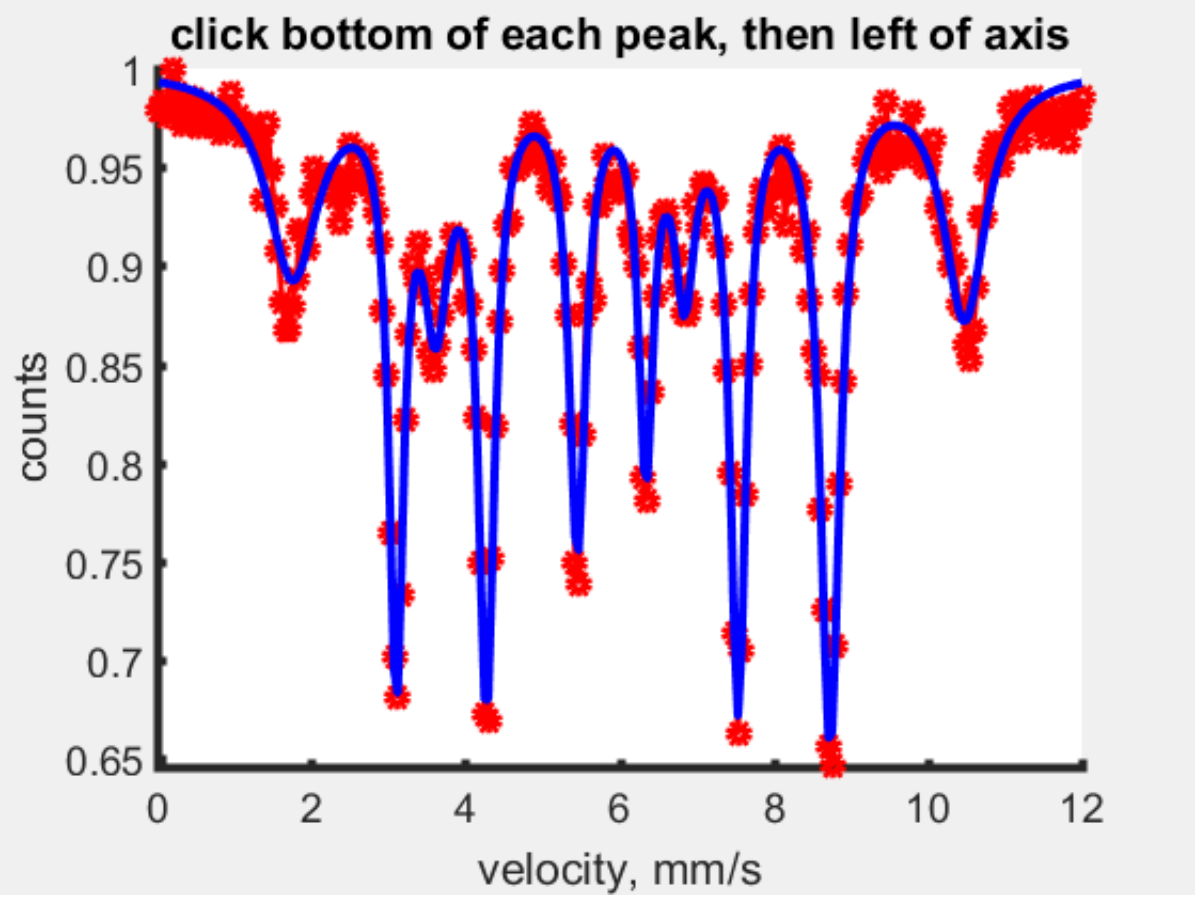
```


% input peaks
```

```
MAXPEAKS=100;
a = zeros(MAXPEAKS,1);
v0 = zeros(MAXPEAKS,1);
c = zeros(MAXPEAKS,1);
K=0;
for k = [1:20]
    p = ginput(1);
    if( p(1) < 0 )
        break;
    end
    K=K+1;
    a(K) = p(2)-A;
    v0(K)=p(1);
    c(K)=0.1;
end
a = a(1:K);
v0 = v0(1:K);
c = c(1:K);

% model parameters
M=K*3;
m = [a', v0', c']';

for iter=[1:10]

dpre = A*ones(N,1);
for i = [1:K]
    temp = ((v-m(K+i)).^2+m(2*K+i)^2);
    dpre = dpre + m(i)*(m(2*K+i)^2)./temp;
end

% data kernel
G=zeros(N,M);
for i = [1:K]
    temp = ((v-m(K+i)).^2+m(2*K+i)^2);
    G(:,i) = (m(2*K+i)^2)./temp; % d/da
    G(:,K+i) = 2*m(i)*(m(2*K+i)^2)*(v-m(K+i))./(temp.^2);  % d/dv0
    G(:,2*K+i) = 2*m(i)*m(2*K+i)./temp - 2*m(i)*m(2*K+i)^3./(temp.^2);  % d/dc
end

% deviations in data
dd = d - dpre;
E = dd'*dd;

% updated model
dm = (G'*G+0.001*eye(M))\(G'*dd);
mold=m;
m = m+dm;

disp(sprintf('%f', E));

end
```

```
0.303583
0.102488
0.041978
0.039029
0.038614
0.038530
```

```
0.038509
0.038504
0.038503
0.038502
```

```
% plot
dpre2 = A*ones(N,1);
for i = [1:K]
    temp = ((v-m(K+i)).^2+m(2*K+i)^2);
    dpre2 = dpre2 + m(i)*(m(2*K+i)^2)./temp;
end
plot(v,dpre2,'b-','LineWidth',3);
```




```
% Figure 1.4 Example of a Mossbauer spectroscopy experiment performed by the Spirit rover
% on Martian soil. (Red) Absorption peaks reflect the concentration of different iron-bearing
% minerals in the soil. The inverse problem is to determine the position and area of each peak
% which can be used to determine the concentration of the minerals. (Blue) The sum of ten
% Lorentzian curves fit to the data. Data courtesy of NASA and the University of Mainz. MatLab
% script gda01_04.
```