University of Helsinki / Department of Mathematics and Statistics
SCIENTIFIC COMPUTING
Exercise 12 / Solutions

1. Show experimentally that for real 2×2 matrices A=[a b; c d] the following equality holds;

$$cond(A) = s + \sqrt{s^2 - 1} \quad \text{where} \quad s = (a^2 + b^2 + c^2 + d^2)/(2|\det(A)|).$$

Solution:

```
% FILE: d121.m begins
% Forsythe-Moler p. 25 says that if A=[a b; c d] satisfies
% det(A)=ad-bc not zero and s= (a*a+b*b+c*c+d*d)/(2*det(A))
% then cond(A)= s + sqrt(s*s-1)
n=2;
fprintf('d121:  Error\n')
for p=1:15
  A=3*(rand(n,n)-0.5);
  t= norm(A(:)')^2;
  s=t/(2*abs(det(A)));
  tmp=cond(A)-s-sqrt(abs(s*s-1));
  fprintf('% 12.2e\n',tmp)
end
% FILE: d121.m ends
```

Output:

```
d121:  Error
   -2.22e-16
    3.33e-16
    4.44e-16
   -6.66e-16
    4.44e-16
   -1.22e-15
    6.66e-16
   -3.20e-13
    9.44e-16
   -7.46e-14
    1.78e-15
   -6.66e-16
    3.11e-15
   -4.44e-16
   -1.22e-15
```

2. Use the data d122dat.dat to fit the model $f(\lambda_1, \lambda_2, \lambda_3, x) = \lambda_1/(1 + (x - \lambda_2)^2) + 1/(1 + (x - \lambda_3)^2)$. Use the initial values [1,-1,2] as a guess. Hint: parfit or parf04.

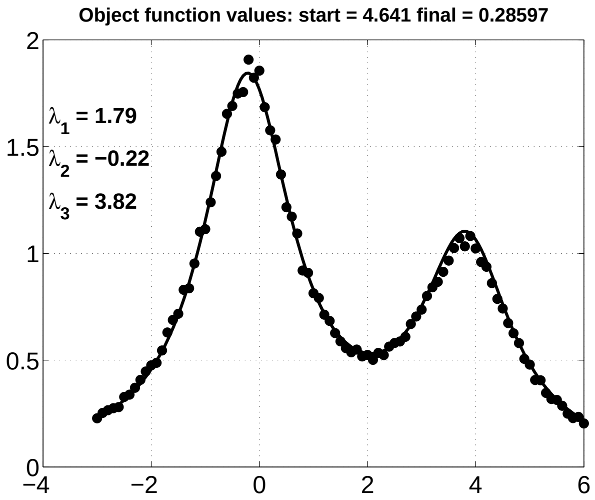
Solution:

```
% FILE d122.m begins.
% Uses modified parfit, see d083.m and d062rajala.m
fmodel =...
 inline('lam(1)./(1+(x-lam(2)).^2)+1./(1+(x-lam(3)).^2)','x','lam');
fobj =...
 inline('norm(feval(fmodel,x,lam) - y)', 'lam','fmodel','x','y');

load d122dat.dat ;   xdat=d122dat(:,1)';     ydat=d122dat(:,2)';
lam0=[1 -1 2];
y0=fobj(lam0,fmodel,xdat,ydat);   % Initial value of object function
lam=fminsearch(fobj,lam0,[],fmodel,xdat,ydat);
fprintf('d122:\n lam= '); fprintf('  %f',lam); fprintf('\n');
                        % lam is the fitted value for
                        % the parameter vector
x=min(xdat):0.05:max(xdat);
yfit=fmodel(x,lam);
yfinal=fobj(lam,fmodel,xdat,ydat);% Final value of the object function
figure(1)
axes('FontWeight','bold','FontSize',20);
plt=plot(x,yfit,xdat,ydat,'k.','MarkerSize',25);  grid on;
title(['Object function values: start = ' num2str(y0) ...
                              ' final = ' num2str(yfinal)],...
      'FontWeight','bold','FontSize',16);
ax=axis;
text(ax(1)+0.1,ax(4)-0.4,...
     ['\lambda_1 = ' num2str(lam(1),'%5.2f')],...
     'FontWeight','bold','FontSize',18);
text(ax(1)+0.1,ax(4)-0.6,...
     ['\lambda_2 = ' num2str(lam(2),'%5.2f')],...
     'FontWeight','bold','FontSize',18);
text(ax(1)+0.1,ax(4)-0.8,...
     ['\lambda_3 = ' num2str(lam(3),'%5.2f')],...
     'FontWeight','bold','FontSize',18);
set(plt,'LineWidth',2.5);
% FILE d122.m ends.
```

Output:

```
d122:
```

```
lam=   1.786561  -0.221072  3.822403
```



Alternative solution:

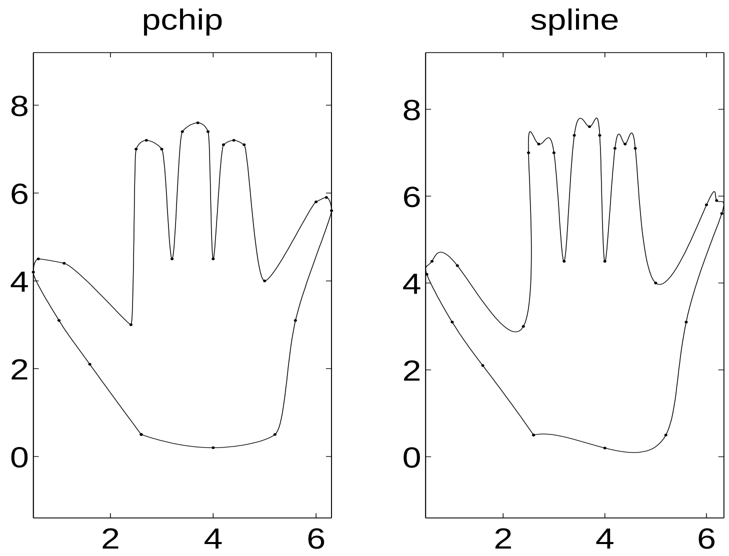
```
function d122
data = load('d122dat.dat');
xdata = data(:,1); ydata = data(:,2);

fobj = @(lam) norm(fmodel(lam,xdata)-ydata);
lam0 = [1,-1,2];
lam = fminsearch(fobj,lam0);

figure(1);
clf;
axes('FontSize',[14],'FontWeight','bold');
hold on;
x = -4:.01:7;
plot(x,fmodel(lam,x),'b','LineWidth',2.5);
plot(xdata,ydata,'r+');
legend('sovitus','aineisto');
txt = sprintf('y = %5.5f/(1+(x-%5.5f)^2)+1/(1+(x-%5.5f)^2)',lam(1),lam(2),lam(3));
title(txt);
hold off;

function res = fmodel(lam,x);
res = lam(1)./(1+(x-lam(2)).^2)+1./(1+(x-lam(3)).^2);
```


3. The program hlp123.m on the www-page plots a curve through given points. Use it to plot the shape of your hand using sufficiently many points, e.g.25-30 points. Experiment with the program by changing pchip to spline and other methods of interpolation.

Solution:

```
% FILE d123.m begins.
clear
close all
x=[2.6 1.6 1.0 0.5 0.6 1.1 2.4 2.5 2.7 3.0 3.2  3.4 3.7 ...
3.9 4.0 4.2 4.4 4.6 5.0 6.0 6.2 6.3 5.6 5.2 4.0 2.6];
y=[0.5 2.1 3.1 4.2 4.5 4.4 3.0 7.0 7.2 7.0 4.5 7.4 7.6 ...
7.4 4.5 7.1 7.2 7.1 4.0 5.8 5.9 5.6 3.1 0.5 0.2 0.5];
m=length(x);
xi =1:0.05:m;
pi=interp1(1:m,x,xi,'pchip');
qi=interp1(1:m,y,xi,'pchip');
subplot(1,2,1)
plot(x,y,'r.',pi,qi,'b-')
title(['pchip'])
axis('equal')
xi =1:0.05:m;
pi=interp1(1:m,x,xi,'spline');
qi=interp1(1:m,y,xi,'spline');
subplot(1,2,2)
plot(x,y,'r.',pi,qi,'b-')
title('spline')
axis('equal')
% FILE d123.m ends.
```

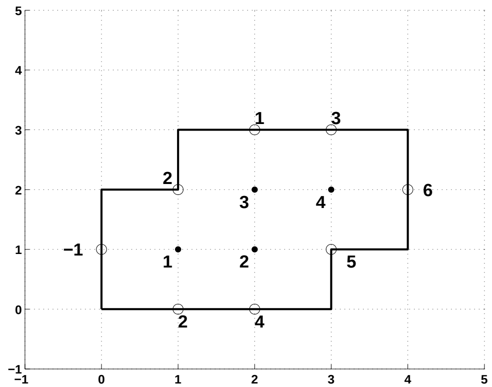
Output:



4. Solve Dirichlet's problem

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

in the situation pictured below, by using the boundary values and the numbering of variables as in the picture. The sidelength of a square is 1.



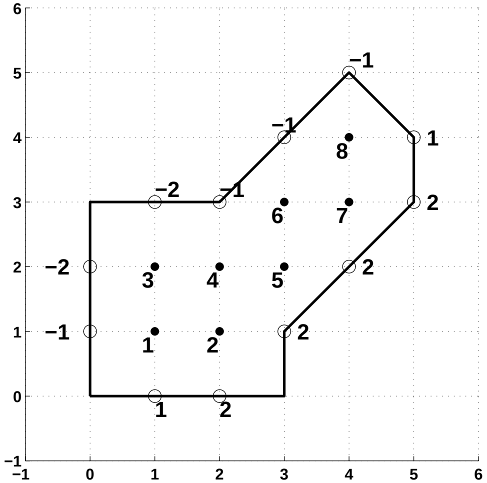
Solution:

```
% FILE d124.m begins
close all;
%clear all;
clc;
%                            % b
% 4*p1 = -1 + 2 + p2 + 2;    % 3
% 4*p2 = p1 + p3 + 5 + 4;    % 9
% 4*p3 = 2 + 1 + p4 + p2;    % 3
% 4*p4 = p3 + 3 + 6 + 5;     % 14
a = [ 4 -1 0 0;
     -1 4 -1 0;
     0 -1 4 -1;
     0 0 -1 4];
b = [ 3 9 3 14];
disp([a b'])
t = a\b'
% FILE d124.m ends.
```

Output:

```
     4    -1     0     0     3
    -1     4    -1     0     9
     0    -1     4    -1     3
     0     0    -1     4    14


t =

    1.5742
    3.2967
    2.6124
    4.1531
```

5. As 4, but in the situation of the following picture.



Solution:

```
% FILE: d125.m begins
%clear all;
close all; clc;
%                               % b
% 4*p1 = -1 + p3 + p2 +1;      % 0
% 4*p2 = p1 + p4 + 2 + 2;      % 4
% 4*p3 = -2 + -2 + p4 + p1;    % -4
% 4*p4 = p3 + -1 + p5 + p2;    % -1
% 4*p5 = p4 + p6 + 2 + 2;      % 4
% 4*p6 = -1 + -1 + p7 + p5;    % -2
% 4*p7 = p6 + p8+ 2 + 2;       % 4
% 4*p8 = -1 + -1 + 1 + p7;     % -1
a = [ 4 -1 -1 0 0 0 0 0;
     -1 4 0 -1 0 0 0 0;
     -1 0 4 -1 0 0 0 0;
     0 -1 -1 4 -1 0 0 0;
     0 0 0 -1 4 -1 0 0;
     0 0 0 0 -1 4 -1 0;
     0 0 0 0 0 -1 4 -1;
     0 0 0 0 0 0 -1 4];
b = [0 4 -4 -1 4 -2 4 -1];
disp([a b'])
t = a\b'
% FILE: d125.m ends
```


Output:

```
     4    -1    -1     0     0     0     0     0     0
    -1     4     0    -1     0     0     0     0     4
    -1     0     4    -1     0     0     0     0    -4
     0    -1    -1     4    -1     0     0     0    -1
     0     0     0    -1     4    -1     0     0     4
     0     0     0     0    -1     4    -1     0    -2
     0     0     0     0     0    -1     4    -1     4
     0     0     0     0     0     0    -1     4    -1


t =

   -0.0000
    1.0000
   -1.0000
   -0.0000
    1.0000
   -0.0000
    1.0000
         0
```

6. Consider the data $(x_j, y_j), j = 1, ..., m$, and set

$$f(a,b,c,d,x) = ax^2 + bx + c + d/x\,, \quad S = \sum_{j=1}^{m} (y_j - f(a,b,c,d,x_j))^2\,.$$

A researcher is modelling the political awareness in EU countries using this model.

(a) Help the researcher to set up the normal equations. (Recall that these are $\frac{\partial S}{\partial a} = 0, \frac{\partial S}{\partial b} = 0, \frac{\partial S}{\partial c} = 0, \frac{\partial S}{\partial d} = 0\,.$) Do not solve the normal equations.

(b) Use the method of problem d105 to write the problem in matrix form $X\lambda = Y$, where $X(j,:) = [x_j^2, x_j, 1, 1/x_j], Y(j,1) = y_j$ and $\lambda = [a; b; c; d]$. Then generate synthetic data and use solve this system of equations $\lambda = X \setminus Y$.

Solution:

(a) The normal equations are

$$\frac{\partial S}{\partial a} = 2\sum_{j=1}^{m}\left[ax_j^4 + bx_j^3 + (c-y_j)x_j^2 + dx_j\right] = 0$$
$$\frac{\partial S}{\partial b} = 2\sum_{j=1}^{m}\left[ax_j^3 + bx_j^2 + (c-y_j)x_j + d\right] = 0$$
$$\frac{\partial S}{\partial c} = 2\sum_{j=1}^{m}\left[ax_j^2 + bx_j + (c-y_j) + \frac{d}{x_j}\right] = 0$$
$$\frac{\partial S}{\partial d} = 2\sum_{j=1}^{m}\left[ax_j + b + \frac{(c-y_j)}{x_j} + \frac{d}{x_j^2}\right] = 0.$$

(b)
```
% FILE  d126.m  begins.
% Fit c(1)*x.^2 + c(2)*x + c(3) +c(4)./x  to data
% This program, with small modifications, applies
% also to some other linear problems

close all
clear
for jj=1:5
figure


fmodel=inline('c(1)*x.^2 + c(2)*x + c(3) +c(4)./x ','x','c');
fobj=inline('norm(feval(fmodel,x,c)-y)','c','fmodel','x','y');
% fobj =  sum of squares
xdata= 0.5:0.5:5;
c1=4*rand(4,1)-3*rand(4,1);

y=fmodel(xdata,c1);   % Generate syntetic data
                      % with parameters c1
ydata= y.*(0.97+0.05*rand(1,length(xdata)));
                      % Add some "errors"

xx=xdata'; yy=ydata';
d1=length(xx);
d2=length(c1);
A=zeros(d1, d2);
A=[xx.^2  xx  ones(d1,1) 1./xx];
myc=A\yy;
c=myc';
yfinal=fobj(c,fmodel,xdata,ydata);  % Final value of object function
```

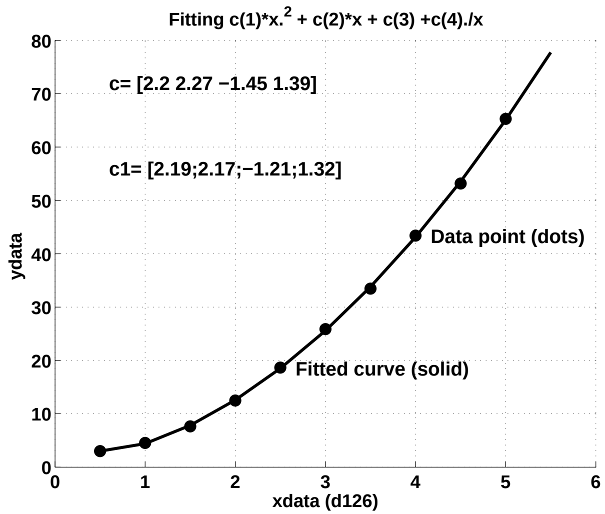


```
fprintf('\nSum of squares = %12.3f \n c1  =',yfinal)
fprintf(' %12.3f ',c1)
fprintf('\ncest =')
fprintf(' %12.3f ',c')
fprintf( '\n')


x=0.5:0.5:5.5;
yfit=fmodel(x, c);

axes('FontSize',[15],'FontWeight','bold'); hold on;
title(['Fitting c(1)*x.^2 + c(2)*x + c(3) +c(4)./x'])
plt=plot(x,yfit,xdata,ydata,'k.','MarkerSize',30);  grid on;
txt1=' {\bf Fitted curve (solid)}';
text(x(5)+0.05,yfit(5),txt1,'FontWeight','bold','FontSize',[16]);
txt2=' {\bf Data point (dots)}';
text(xdata(8)+0.05,ydata(8),txt2,'FontWeight','bold','FontSize',[16]);
ax=axis; x1=ax(1)+0.1*(ax(2)-ax(1));
y1=ax(3)+0.9*(ax(4)-ax(3));
%y1=max(y1,0.5+max(ydata));
text(x1,y1, ['c= ' mat2str(c,3)],'FontWeight','bold','FontSize',[16]);
y2=ax(3)+0.7*(ax(4)-ax(3));
%y2=max(y2,0.3+max(ydata));
text(x1,y2, ['c1= ' mat2str(c1,3)],'FontWeight','bold','FontSize',[16]);
ylabel('ydata '); xlabel('xdata (d126)')
set(plt,'LineWidth',2.5);
pause(1.5)
end
% FILE  d126.m  ends.
```

Output:

```
Sum of squares =       0.929
 c1  =        1.556        3.540        0.063        0.515
cest =        1.452        4.152       -1.103        0.952

Sum of squares =       1.700
 c1  =        3.436        0.066        0.365       -1.043
cest =        3.465       -0.013       -0.023       -0.792

Sum of squares =       1.212
 c1  =        2.176        1.304        2.196        0.514
```

```
cest =        2.331        0.150        4.097       -0.156

Sum of squares =       0.067
 c1  =       -0.379        1.790       -0.340        0.471
cest =       -0.377        1.788       -0.376        0.491

Sum of squares =       0.727
 c1  =        2.192        2.174       -1.209        1.318
cest =        2.197        2.269       -1.448        1.387
```



Alternative solution:

```
g = @(t) [t .^ 2, t, ones(size(t)), 1 ./ t];

x = (1 : 10)';
y = g(x) * [2; 3; 4; 5] + rand(10, 1);

X = g(x);

l = X \ y

f = @(t) g(t) * l;

fprintf('%+e\n', f(x) - y)
fprintf('\n%+e\n', norm(f(x) - y))
```



```
clf
hold on

plot(x, y, 'or', 'MarkerSize', 20)
plot(x, f(x), '-b', 'LineWidth', 2)

hold off
```