

Q3.

## PHY 300/500: Homework 3 Solution

$$\chi^2 = \sum_i \frac{(y_i - mx_i - c)^2}{\alpha_i^2}$$

after experimentation:  $x_i, y_i$  &  $\alpha_i$  are fixed.

i) Show that  $\frac{1}{2} \frac{\partial^2 \chi^2}{\partial c^2} = \sum_i \frac{1}{\alpha_i^2}$

$$\frac{\partial \chi}{\partial c} = \sum_i \frac{-2c}{\alpha_i^2}$$

$$\frac{\partial^2 \chi}{\partial c^2} = \sum_i \frac{2}{\alpha_i^2}$$

$$\boxed{\frac{1}{2} \frac{\partial^2 \chi}{\partial c^2} = \sum_i \frac{1}{\alpha_i^2}}$$

ii) Show that  $\frac{1}{2} \frac{\partial^2 \chi^2}{\partial m \partial c} = \sum_i \frac{x_i}{\alpha_i^2}$

$$\frac{\partial \chi}{\partial m} = \sum_i \frac{2(y_i - mx_i - c) \cdot (-x_i)}{\alpha_i^2}$$

$$\boxed{\frac{1}{2} \frac{\partial^2 \chi}{\partial m \partial c} = \sum_i \frac{x_i}{\alpha_i^2}}$$

iii) Show that  $\frac{1}{2} \frac{\partial^2 \chi^2}{\partial m^2} = \sum_i \frac{x_i^2}{\alpha_i^2}$

$$\frac{\partial \chi}{\partial m} = \sum_i \frac{2(-mx_i) \cdot (-x_i)}{\alpha_i^2}$$

$$\boxed{\frac{1}{2} \frac{\partial^2 \chi}{\partial m^2} = \sum_i \frac{x_i^2}{\alpha_i^2}}$$

$$Q2. \quad C = \begin{bmatrix} \alpha_1^2 & \rho \alpha_1 \alpha_2 \\ \rho \alpha_1 \alpha_2 & \alpha_2^2 \end{bmatrix}$$

$$C^{-1} = \frac{1}{\alpha_1^2 \alpha_2^2 - \rho^2 \alpha_1^2 \alpha_2^2} \begin{bmatrix} \alpha_2^2 & -\rho \alpha_1 \alpha_2 \\ -\rho \alpha_1 \alpha_2 & \alpha_1^2 \end{bmatrix}$$

$$C^{-1} = \frac{1}{1-\rho^2} \begin{bmatrix} \frac{\alpha_2^2}{\alpha_1^2 \alpha_2^2} & \frac{-\rho \alpha_1 \alpha_2}{\alpha_1^2 \alpha_2^2} \\ \frac{-\rho \alpha_1 \alpha_2}{\alpha_1^2 \alpha_2^2} & \frac{\alpha_1^2}{\alpha_1^2 \alpha_2^2} \end{bmatrix}$$

$$C^{-1} = \frac{1}{1-\rho^2} \begin{bmatrix} \frac{1}{\alpha_1^2} & -\frac{\rho}{\alpha_1 \alpha_2} \\ -\frac{\rho}{\alpha_1 \alpha_2} & \frac{1}{\alpha_2^2} \end{bmatrix}$$

$$C(I-\lambda) = \begin{bmatrix} \alpha_1^2 - \lambda & \rho \alpha_1 \alpha_2 \\ \rho \alpha_1 \alpha_2 & \alpha_2^2 - \lambda \end{bmatrix}$$

$$0 = \det = \alpha_1^2 \alpha_2^2 - \alpha_1^2 \lambda - \alpha_2^2 \lambda + \lambda^2 - \rho^2 \alpha_1^2 \alpha_2^2$$

$$\lambda^2 - (\alpha_1^2 + \alpha_2^2) \lambda + \alpha_1^2 \alpha_2^2 (1 - \rho^2) = 0$$

$$\lambda_{\pm} = \frac{1}{2} (\alpha_1^2 + \alpha_2^2) \pm \sqrt{(\alpha_1^2 + \alpha_2^2)^2 - 4 \alpha_1^2 \alpha_2^2 (1 - \rho^2)}$$

$$\begin{bmatrix} \alpha_1^2 & \rho \alpha_1 \alpha_2 \\ \rho \alpha_1 \alpha_2 & \alpha_2^2 \end{bmatrix} \begin{bmatrix} \cos \phi \\ \sin \phi \end{bmatrix} = \lambda \begin{bmatrix} \cos \phi \\ \sin \phi \end{bmatrix}$$

$$\alpha_1^2 \cos \phi + \rho \alpha_1 \alpha_2 \sin \phi = \lambda \cos \phi$$

$$\rho \alpha_1 \alpha_2 \cos \phi + \alpha_2^2 \sin \phi = \lambda \sin \phi$$

$$\alpha_1^2 \cos \phi + \rho \alpha_1 \alpha_2 \sin \phi = \frac{\rho \alpha_1 \alpha_2 \cos \phi + \alpha_2^2 \sin \phi}{\sin \phi} \cos \phi$$

$$\alpha_1^2 + \rho \alpha_1 \alpha_2 \frac{\sin \phi}{\cos \phi} = \rho \alpha_1 \alpha_2 \frac{\cos \phi}{\sin \phi} + \alpha_2^2$$

$$\alpha_1^2 + \rho \alpha_1 \alpha_2 \tan \phi = \frac{\rho \alpha_1 \alpha_2}{\tan \phi} + \alpha_2^2$$

$$\alpha_1^2 - \alpha_2^2 = \frac{\rho \alpha_1 \alpha_2}{\tan \phi} - \rho \alpha_1 \alpha_2 \tan \phi$$

$$\alpha_1^2 - \alpha_2^2 = \rho \alpha_1 \alpha_2 \left[ \frac{1 - \tan^2 \phi}{\tan \phi} \right]$$

$$\frac{(\alpha_1^2 - \alpha_2^2)}{2\rho \alpha_1 \alpha_2} = \frac{1}{\tan 2\phi}$$

$$\boxed{\tan 2\phi = \frac{2\rho \alpha_1 \alpha_2}{\alpha_1^2 - \alpha_2^2}}$$

7.8  
Q4.

↓ Comes from 7.7

$$\frac{1}{2} A = \begin{bmatrix} \frac{1}{2} \frac{\partial^2 X}{\partial c^2} & \frac{1}{2} \frac{\partial^2 X}{\partial m \partial c} \\ \frac{1}{2} \frac{\partial^2 X}{\partial c \partial m} & \frac{1}{2} \frac{\partial^2 X}{\partial m^2} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \sum_i \frac{1}{\alpha_i^2} & \sum_i \frac{x_i}{\alpha_i^2} \\ \sum_i \frac{x_i}{\alpha_i^2} & \sum_i \frac{x_i^2}{\alpha_i^2} \end{bmatrix} = \begin{bmatrix} 100 & 70 \\ 70 & 8.75 \end{bmatrix}$$

$$A^{-1} = \frac{1}{(100)(8.75) - (70)(70)} \begin{bmatrix} 8.75 & -70 \\ -70 & 100 \end{bmatrix} = \begin{bmatrix} 7.14 \times 10^{-3} & -0.05712 \\ -0.05712 & 0.5712 \end{bmatrix}$$

Correlation matrix:

$$\rho_{AB} = \frac{\sigma_{AB}}{\sigma_A \sigma_B} = \frac{C_{AB}}{\sqrt{C_{AA} C_{BB}}} = \begin{bmatrix} \frac{7.14 \times 10^{-3}}{\sqrt{(7.14 \times 10^{-3})^2}} & \frac{0.05712}{\sqrt{(7.14 \times 10^{-3})(0.5712)}} \\ \frac{0.05712}{\sqrt{(7.14 \times 10^{-3})(0.5712)}} & \frac{0.5712}{\sqrt{(0.5712)^2}} \end{bmatrix}$$

$$\rho = \begin{bmatrix} 1 & -0.8944 \\ -0.8944 & 1 \end{bmatrix}$$

$$i) u_{\text{int}} = \sqrt{7.14 \times 10^{-3}} = 0.0845$$

$$u_{\text{grad}} = \sqrt{0.5712} = 0.7558$$

$$ii) y = mx + c$$

$$y = (431.7)(0.08) + (-0.03)$$

$$y = 34.506$$

In[30]= Question 1

```
Clear["Global`*"]
```

```
noise = {};  
values = Table[5 Exp[-0.2 var], {var, 0, 10, 0.2}];  
var = Range[0, 10, 0.2];
```

```
For[i = 1, i < 52, i++, AppendTo[noise, RandomVariate[NormalDistribution[0, 0.2]]]]  
noisydata = values + noise;
```

```
idealdata = a Exp[-b var];  
chisquare1 = Expand[Sum[ $\frac{(\text{idealdata}[[n]] - \text{noisydata}[[n]])^2}{0.2^2}$ , {n, 1, 51}]];  
gradχsq = -Grad[chisquare1, {a, b}];  
H = {{D[D[chisquare1, a], a], D[D[chisquare1, a], b]},  
     {D[D[chisquare1, b], a], D[D[chisquare1, b], b]}};  
diagH = DiagonalMatrix[Diagonal[H]];
```

```
arraychisquare1 = {};  
arraychisquare2 = {};  
steparray = {};
```

```
vec = {8, 3};  
vec2 = {};  
step = 0.01;
```

```
For[i = 0, i < 50, i++,  
  chisquare1 = Expand[Sum[ $\frac{(\text{idealdata}[[n]] - \text{noisydata}[[n]])^2}{0.2^2}$ , {n, 1, 51}]];  
  H = {{D[D[chisquare1, a], a], D[D[chisquare1, a], b]},  
       {D[D[chisquare1, b], a], D[D[chisquare1, b], b]}};  
  diagH = DiagonalMatrix[Diagonal[H]];  
  gradχsq = -Grad[chisquare1, {a, b}];
```

```
  a = vec[[1]];  
  b = vec[[2]];  
  chisquare2 = chisquare1;  
  AppendTo[arraychisquare2, chisquare2];
```

```
variation = -Inverse[H + (step diagH)].gradχsq;
```

```

vec = vec + variation;

Clear[a, b, chisquare1];
chisquare1 = Expand[Sum[ $\frac{(\text{idealdata}[[n]] - \text{noisydata}[[n]])^2}{0.2^2}$ , {n, 1, 51}]];
a = vec[[1]];
b = vec[[2]];

AppendTo[arraychisquare1, chisquare1];
AppendTo[steparray, step];
AppendTo[vec2, vec];

a = vec[[1]];
b = vec[[2]];

If[chisquare1 > chisquare2, step = step * 10; vec = vec - variation, step =  $\frac{\text{step}}{10}$ ];

Clear[a, b, chisquare1, chisquare2];
]

vec2;
steparray;
arraychisquare1;
arraychisquare2;
a = vec[[1]]
b = vec[[2]]
fit = Table[a Exp[-b var], {var, 0, 10, 0.2}];

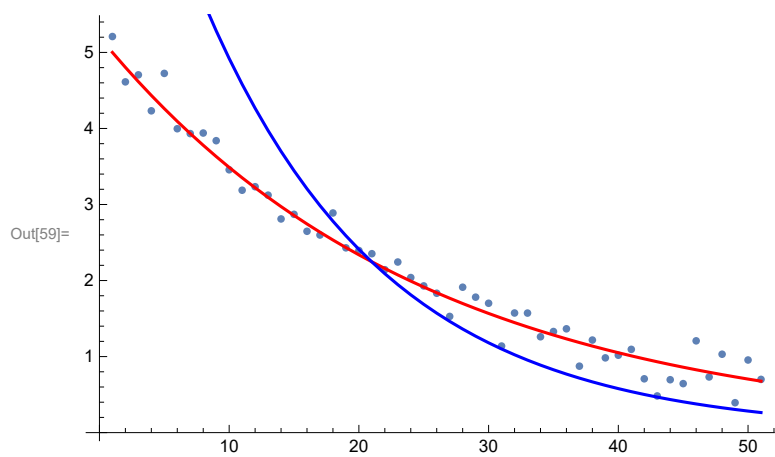
plot1 = ListPlot[noisydata];
plot2 = ListLinePlot[values, PlotStyle -> Red];
plot3 = ListLinePlot[fit, PlotStyle -> Blue];
Show[plot1, plot2, plot3]

```

Out[30]= Question

Out[53]= 9.3508

Out[54]= 0.356726



\*\*\*\*\*Question 1. (Alternate) [MATLAB]\*\*\*\*\*

```
A1=5;
B1=2e-1;
xdata=0:0.1:10;
randstrength=0.1;
ydata=A1*exp(-B1*xdata)+randstrength*randn(1,length(xdata));
figure; plot(xdata,ydata);
kmax=1000;
u=0.1; %uncertainty in each measurement

x=[1;0.02]; %initial value of the parameters

chi2_initial=sum((ydata-x(1)*exp(-x(2)*xdata)).^2/u.^2);
chimatrix=chi2_initial;
xmatrix=x;

slopex=zeros(2,1);
M=zeros(2,2); %M is our Hessian matrix
beta=0.00001;

%implementing the Levenberg-Marquart method

k=0;
deltachiabs=5;

while deltachiabs>1e-10
    k=k+1;
    %computing the gradient
    slopex1=2/u^2*sum(exp(-2*x(2)*xdata).*(x(1)-ydata.*exp(x(2)*xdata)));
    slopex2=2/u^2*sum(x(1)*exp(-2*x(2)*xdata).*xdata.*(-x(1)+ydata.*exp(x(2)*xdata)));
    slopex=[slopex1;slopex2];

    %computing the Hessian matrix
    M(1,1)=2/u^2*sum(exp(-2*x(2)*xdata));
    M(1,2)=2/u^2*sum(exp(-2*x(2)*xdata).*xdata.*(-2*x(1)+ydata.*exp(x(2)*xdata)));
    M(2,1)=M(1,2);
    M(2,2)=-2/u^2*sum(x(1)*exp(-2*x(2)*xdata).*xdata.^2.*(-2*x(1)+ydata.*exp(x(2)*xdata)));
    Mtemp=(M+beta*diag(diag(M)));
    Mtemp1=1/(Mtemp(1,1)*Mtemp(2,2)-Mtemp(1,2)*Mtemp(2,2))*[Mtemp(2,2) -Mtemp(1,2); -Mtemp(2,1) Mtemp(1,1)];

    xa=x; %current parameters
    xb=x-Mtemp1*slopex; %proposed paramaters

    chia=sum((ydata-xa(1)*exp(-xa(2)*xdata)).^2/u.^2);
    chib=sum((ydata-xb(1)*exp(-xb(2)*xdata)).^2/u.^2); %proposed chi^square

    deltachitest=chib-chia;
    deltachiabs=abs(chib-chia);

    if deltachitest >= 0
        beta=beta*10;
        xmatrix=[xmatrix xa];
```



```

chimatrix=[chimatrix chia];
x=xa;
chi=chia;

else
    beta=beta/10;
    xmatrix=[xmatrix xb];
    chimatrix=[chimatrix chib];
    x=xb;
    chi=chib;
end

fprintf('i=%d, A=%f, B=%f, chi=%.3f dchitest=%e beta=%f \n', ...
k, x(1),x(2),chi, deltachiabs, beta);
end

*****QUESTION 5*****
angled=0:10:270;
angle=angled*pi/180;
lengthdata=length(angle);
intensity=0.5*cos(0.9*angle+0.6).^2-0.3+0.03*randn(1,lengthdata);
figure; plot(angle,intensity,'o');
u=[0.0005*ones(1,lengthdata)];

x=[1; 2; -1; 0]; %initial guess of the parameters
chi=sum((intensity-(x(1)+x(2)*cos(x(3)*angle+x(4)).^2)).^2/u.^2);
T=1000; %initial temperature

for k=1:1000
    xa=x;
    Ea=sum((intensity-(xa(1)+xa(2)*cos(xa(3)*angle+xa(4)).^2)).^2/u.^2);
    xb=x+0.1*randn(4,1);
    Eb=sum((intensity-(xb(1)+xb(2)*cos(xb(3)*angle+xb(4)).^2)).^2/u.^2);
    DE=Eb-Ea;
    if Eb<Ea
        x=xb;
    else
        R=rand;
        P=exp(-DE/T);
        if P>R
            x=xb;
        else
            x=xa;
        end
    end

    end
    T=T-0.01*T;
    fprintf('i=%d, T=%.7f, chi=%f, A=%f, B=%f, C=%f, D=%f, \n', ...
k, T, Ea, x(1), x(2), x(3), x(4) );

end

figure; plot(angle,intensity,'o');

```

```
hold on;  
plot(angle,x(1)+x(2)*cos(x(3)*angle+x(4)).^2);  
hold off;
```