
```

%HW1-Prb6
%Navneet Singh(nsinghl@andrew.cmu.edu)

% lnK = lnKo - (1/RT)*Ea , here we have two unknowns Ko and Ea.
%We have been given 5 values of K and T. So we have 2 unknowns and
% 5 equations. So this a problem of overdeterminant system. This can
be
% solved by least square systems. After conevrting equation to Ax = b
form
% x = [inv(A'A)*A']*b.

clc          %clear screen
clear all    %clearing all stored variables
close all    %close previous plots

%Initializing given variables
R = 8.314;                                %J/K
T = [430, 450, 470, 480, 490]';          %K
k = [0.0026, 0.0118, 0.0460, 0.0873, 0.1800]'; %s-1

b = log(k); % Generating vector b. we have taken natural log on both
sides to model this as a linear problem.

%Initializing Matrix A
A = zeros(5,2);
A(:,1) = 1.0; %first column of matrix A
A(:,2) = (-1)./(R.*T); %second column of matrix A

x = (inv(A'*A)*A')*b ; %solving unknowns using pseudoinverse of A.

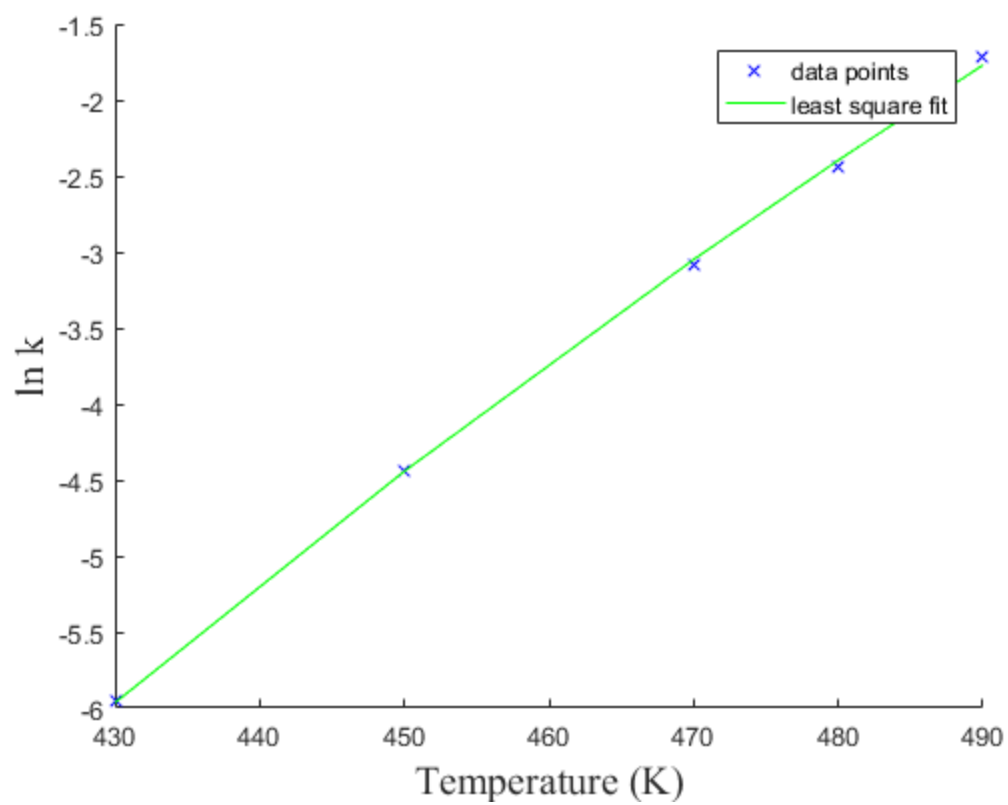
ko = exp(x(1)); % calculating value pre-exponential factor, ko.
Ea = x(2); % calculating activation energy, Ea.
fprintf('Pre exponential factor, Ko = %d sec^-1 \n',ko)
fprintf('Activation Energy, Ea = %d J \n',Ea)

ls = x(1) - Ea./(R.*T); %calculating least square fit of data.

hold on
plot(T,b,'bx') %plotting data points.
plot(T,ls,'g-') %plotting least square fit.
legend('data points','least square fit')
xlabel('Temperature (K)','fontsize',15,'fontname','times new roman')
ylabel('ln k','fontsize',15,'fontname','times new roman')

Pre exponential factor, Ko = 1.949209e+12 sec^-1
Activation Energy, Ea = 1.224946e+05 J

```



Published with MATLAB® R2016a