IIT Madras

ONLINE DEGREE

Mathematics for Data Science 1
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Indian Institute of Technology, Madras Week 9 Tutorial

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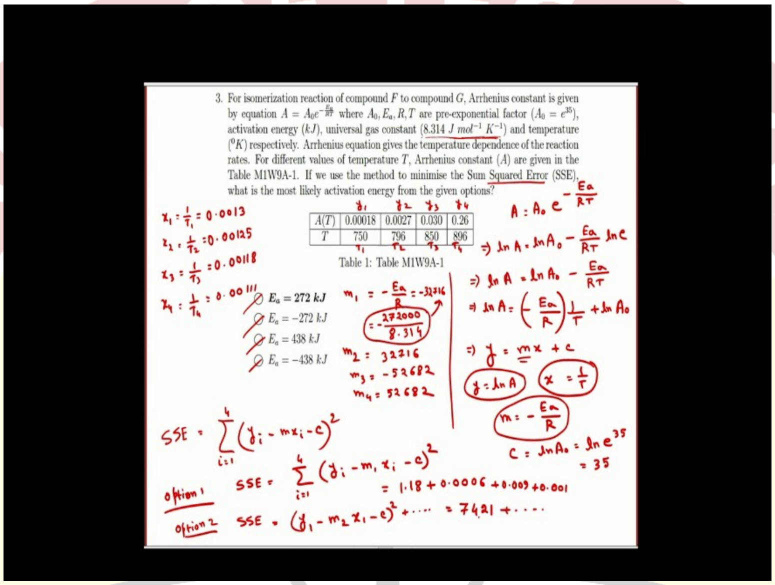

So, let us see what the third question is. So, the third question says that for isomerization reaction of compound F to compound G, Arrhenius constant is given by the equation $A = A_0 e^{\frac{E_A}{RT}}$ T, where A_0, E_A, R and T are pre-exponential factor and A_0 is given as e^{35} which is the activation energy, universal gas constant which is R, this R is universal gas constant, temperature is T, then Arrhenius equation gives the temperature dependence of the reaction rates, for different values of temperature T, Arrhenius constant A are given in the table, so for different T's, this given AT's given.

So, if we use the method to minimize the sum square error, which is SSE, what is the most likely activation energy from the given options? So, E_A is the activation energy, so let us see what this thing says. So, you can take log on both sides, so log we are taking as base as e so I am using this notation ln and here also this term will come before $ln\ e$, so this will be our equation, if we take log. So, this will give us this $ln\ e$ is 1, so $\frac{E_A}{RT}$, so we can write it like this way.

So, this is in the form $y = mx + c$, where y is ln A which is our dependent variable, x is $\frac{1}{T}$which is the independent variable, m is the slope which is given as $\frac{E_A}{R}$ and our constant c is ln of $\ln A_0$, now A_0 is given as e^{35}, so it will be e^{35}, which is nothing but 35, so c is 35.

So, we are taking x as $\frac{1}{T}$, so these are T_1, T_2, T_3 and T_4, so we can write calculate what our xi's, so $x1$ is $x_1 = \frac{1}{T_1}$ which will get if we calculate will get 0.0013, you can do the calculation by yourself, so I am just writing this values, so these are 4 values of xi, where i runs from 1 to 4. So, what we have to calculate to calculate the SSC? So, for different xi you will get different yi using this equation where m is m will vary depending on these four options.

So, there are four possible ways, so let us write this for option 1, I am writing it as m1, so if we calculate m1 which is $\frac{-E_A}{R}$ and I am taking the first E_A first option 272 as my first E_A, so I am getting-32716, so what we are doing here E_A is given as 272 kilojoule but this you can observe that the universal gas constant is given as joule mol inverse and Kelvin inverse, so basically for E_A 272 we have to take 272000, so this we have to convert it in terms of joule and then we have to divide it with the universal gas constant which is 8.314 and there is a minus, so if we calculate this then you will get this one.

Similarly, you can calculate m_2 as 32716, m_3 as-52682 and m_4 as 52682. So, these are the four possibilities for m_1, m_2, m_3, and m_4. Now see what SSE is. So, SSE is basically some square error, so if I put different values of x_i we will get different y and the error will be this y_i-that y which are we getting by putting different x_i. So, the error will be $y_i - mx_i - c$, we have to take the square of the error because this is squared error and we have to take sum of this, so this is our SSE, i=1 to 4, so this is the formula for SSE.

Now, here for different option we are getting different mi, so SSE for option 1, so for 4 different option we have to calculate the SSE and we have to see which one is the minimum. So, SSE for option 1 will be $\sum_{i=1}^{4}(y_i - m_1x_i - c)^2$. So, you have to just put this x_i, put the first m_1 here, c is same for all the terms, so which is 35 and you have to subtract that from this y_i and take the square of it and take the sum of it.

So, if you calculate this, you will see the first the first one you will get something like 1.18+0.0006+0.009+0.001 and if we calculate for the second option for the second option you will see the first term the first term alone which is $(y_2 - m_2 x_1 - 3)^2$ +there are three more term, so the first time alone will give you 7421 and there are three more term and all these terms are positive because these are square. So, it is definitely greater than the first option.

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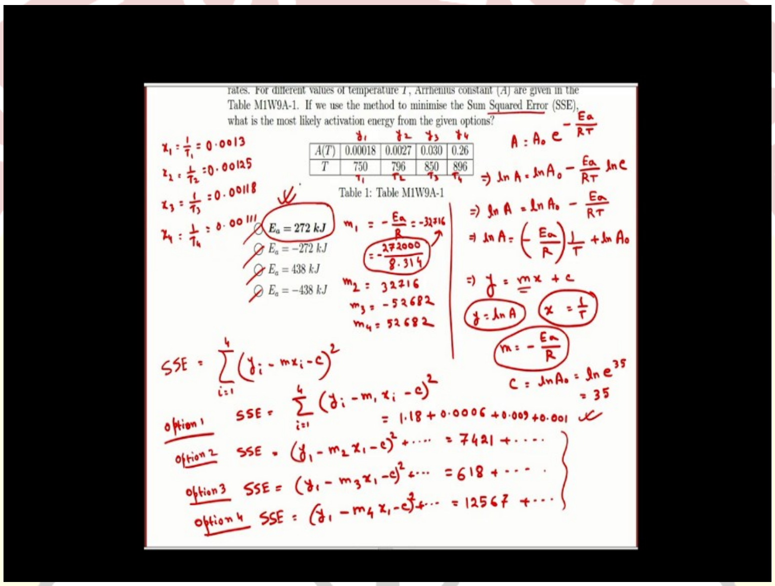

Now, again if we calculate for option 3 again you will see the first term we will be 618 and there are some 3 more terms if we calculate option 4 and observe only the first term you will get 12567 and some 3 more times. So, observe that all these terms are much greater than this option 1, so option 1 will give you the list SSE. So, option 1 is the correct option.