4 Mostly optimization

Group 1

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I hereby declare that all solutions are entirely my own work, without having taken part of other solutions.

The number of hours spent: 20hours (Min Wu)

The number of hours has been present in supervision for this module: 3h (keeping track)

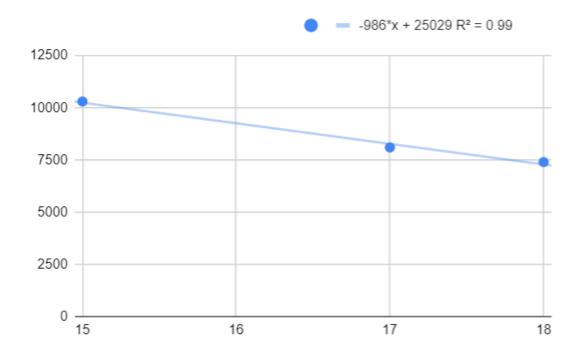
1. (WHAT IS THE REVENUE?)

Consider this data for sales and pricing of chocolate bars:

year	quantity	unit price
2014	10300	15 kr
2015	8100	17 kr
2016	7400	18 kr

a) Assuming that this data gives an indication of the price sensitivity of chocolate bar sales, how can you estimate a) for which price revenue is maximized, b) for which price profit is maximized, if we have a production cost of 3 kr per bar (ignoring fixed costs). Perform any calculations as far as possible.

a)The price vs quantity is plotted, see the following.



The relationship between price and quantity is likely linked to a linear function y=ax+b. The equation can be solved by the two known data (15,10300) and (18, 7400). The function is thus quantity = -986* price + 25029 with R^2=0.99.

The income will be the quantity * price: income=quantity*price

2014 income: 10,300*15 kr =154,500 kr 2015 income: 8,100*17 kr= 137,700kr 2016 income: 7,400*18 kr= 133,200kr

Income = quantity*price, which quantity= -986*price +25,029.

The relationship between income and price then become:

Income =-986*price^2+25,029*price.

The maximum can be solved when derivative of income is equal to 0.

the derivative income:

income'= -1,972*price+25,029

then income'=0:

-1,972*price +25,029=0 price=12.7 kr

Conclusion: when the price is set to 12.7kr, the revenue is maximized and it is 158,836kr

```
b) Profit = quantity * (price - production cost)
```

= quantity * (price-3)

The relationship between profit and quantity, the profit become:

Profit = (-986*price+25,029)*(price-3)

= -986 * price ^2 + 27,987* price - 75,087

The maximum profit can be obtained when the derivative of profit equals 0

Derivative of profit:

Profit'=-1,972 * price + 27,987

Profit'=0

-1,972*price+27,987=0

price = 14.2 kr

Conclusion: when the price is set to 14.2 kr the profit is maximized and it is 123, 511.4kr

b) Even though you do not know much about the specific situation, hypothesize other possible reasons for the decline in chocolate bar sales.

The price of candy is decreased, so more people tended to buy candy instead of the chocolate bars.

2. (investigating the abstract)

(LEAST SQUARES METHOD)

Fitting a curve graphically can work fine, but there is a limitation in that you then do not have a precise criterion for what is a good fit. The most common criterion in

mathematics is the least squares method (look at any other websites if you like), which minimizes the sum of the squares of the errors between the points and the fitted function. Note how the curve fitting then becomes a well defined optimization problem!

Mathematica uses the least squares criterion in the function Fit, which finds the best linear combination (=weighted sum) of a set of base functions to minimize the quadratic error. For the (EMPIRICAL CURVE FITTING) from the last module, try this out by automatically fitting a quadratic polynomial to the points:

For the quadratic polynomial we use the base functions 1,x and x^2 , and the function will try to fit a linear combination (weighted average) of these functions. So this means that we ask to find a function of the form ax^2+bx+c . Then you can plot with:

```
p1 = ListPlot[data];
p2 = Plot[f, {x, 0, 150000}, PlotStyle -> Red];
Show[p1, p2, PlotRange -> {{0, 150000}, {0, 8000}}]
```

a) As the answer to the question, show the function and the plot.

The function is $185.701+0.0980238 \text{ x}-3.95858*10^-7 \text{ *x}^2$ The plot is

b) Why do you think it may be good to minimize the sum of square errors. Why not simply the sum of the errors for each point?

The error of each point will be positive or negative. The sum of the errors will be zero which indicates no error which is not true.

For example:

error1: 40, error2:-20, error3: -10 and error4: -10

the sum of those errors:

error1+error2+error3+error4=0

But the errors is not zero. By squaring the errors this problem is overcome. The variance is obtained by taking the average of the sum of the squares errors.

3.(SIMPLE ASSIGNMENT PROBLEM)

Take a careful look at how we modelled this problem in the lecture. Try Mathematica for this problem, formulated as a linear programming problem (no integer constraints). Make sure that you understand how the problem is formulated in Mathematica. See what solution you get. Is it fractional or did you get an integer solution?

```
NMinimize[
      \{1 \times 11 + 3 \times 12 + 5 \times 13 + 1 \times 14 + 4 \times 21 + 5 \times 22 + 6 \times 14 + 1 \times 14 + 
3 \times 23 + 2 \times 24 +
                     7 \times 31 + 4 \times 32 + 6 \times 33 + 9 \times 34 + 8 \times 41 + 4 \times 42
+ 7 \times 43 + 3 \times 44
             x11 + x12 + x13 + x14 == 1,
             x21 + x22 + x23 + x24 == 1,
             x31 + x32 + x33 + x34 == 1,
             x41 + x42 + x43 + x44 == 1,
             x11 + x21 + x31 + x41 == 1
             x12 + x22 + x32 + x42 == 1
             x13 + x23 + x33 + x43 == 1,
             x14 + x24 + x34 + x44 == 1
             0 \le x11 \le 1, 0 \le x12 \le 1, 0 \le x13 \le 1, 0
<= x14 <= 1,
             0 \leftarrow x21 \leftarrow 1, 0 \leftarrow x22 \leftarrow 1, 0 \leftarrow x23 \leftarrow 1, 0
<= x24 <= 1,
             0 \le x31 \le 1, 0 \le x32 \le 1, 0 \le x33 \le 1, 0
<= x34 <= 1,
```

```
0 <= x41 <= 1, 0 <= x42 <= 1, 0 <= x43 <= 1, 0
<= x44 <= 1},
    {x11, x12, x13, x14, x21, x22, x23, x24, x31,
    x32, x33, x34, x41,
    x42, x43, x44}
]</pre>
```

To find the minimum

x11+3x12+5x13+x14+4x21+5x22+3x23+2x24+7x31+4x32+6x33+9x34+8x41+4x42+7x4 3+3x44

varibles:

x11,x12,x13,x14,x21,x22,x23,x24,x31,x32,x33,x34,x41,x42,x43,x44

Constraints:

```
x11+x12+x13+x14=1

x21+x22+x23+x24=1

x31+x32+x33+x34=1

x41+x42+x43+x44=1

x11+x21+x31+x41=1

x12+x22+x32+x42=1

x13+x23+x33+x43=1

x14+x24+x34+x44=1

0<=x11,x12,x13,x14,x21,x22,x23,x24,x31,x32,x33,x34,x41,x42,x43,x44<=1
```

Result:

The minimum number is 11

when

```
(x11,1), (x12,0), (x13,0), (x14,0), (x21,0), (x22,0), (x23,1), (x24,0), (x31,0), (x32,1), (x33,0), (x34,0), (x41,0), (x42,0), (x43,0) and (x44,1)
```

x11, x23, x32 and x44 equal 1

the reast variables are 0.

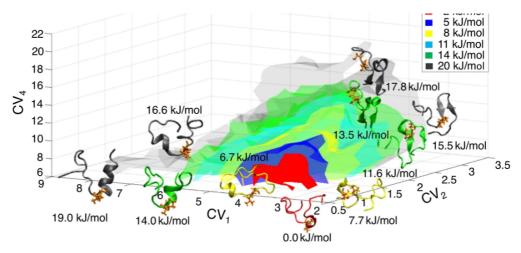
4.(WHEN IS AN OPTIMAL SOLUTION GUARANTEED?)

Numerical optimization algorithms often work with some variant of the following iterative approach:

Make sure to be in a feasible point.

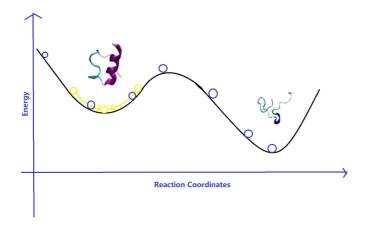
- Take a small step in a direction that will improve the objective function while still staying within the feasible set.
- Repeat until no improvement.

A natural and important question is then if an algorithm of this kind is guaranteed to find the globally optimal solution, or if it is at risk to get stuck in a local optimum. a) Give examples of optimization problems in one and two variables, where this approach will always work, and examples of problems where it may fail. HINT The two-dimensional problem can be seen as finding a highest or a lowest point in a landscape, within a limited geographical area.



The figure above is the 3D-dimensional representation of the free energy landscape of an intrinsically disordered peptide as a function of three collective variables (C1, CV2 and CV4) CV4 is for the number of contacts between the side-chain heavy atoms of different residues. CV1 and CV2 count the number of fragments of 6 residues belonging to α -helix or β -sheet structures respectively.

For an intrinsically disordered protein, for example, an alpha-Synuclein protein which has been identified to play critical roles in Parkinson's Disease. For an intrinsically disordered protein which forms intrinsically disordered structures at the global minimum. However, as the energy increased it forms some relatively stable structures (more beta-sheet or alpha-helix formed structure) at some local minimums which interact with other functional proteins leading to signal transformations or diseases, for example, seeing the figure below:



b) (Voluntary) What is the most general case you can think of, where finding the global optimum can be guaranteed? Consider both the character of the objective function and the shape of the feasible set.

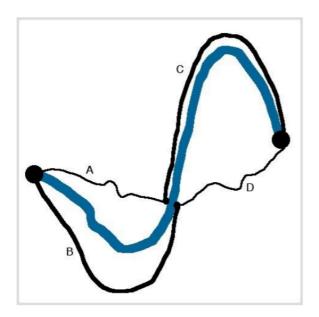
By different starting points which have no relationship between each other and all reactive pathways are calculated together with the constraints, the global optimum is likely to be guaranteed at the lowest point in a landscape.

(investigating the world)

5.(BRIDGE PROBLEM)'

Consider the road network below. The figure illustrates the roads between two larger cities along a river. Roads B and C are large roads and have a fixed travel time of about 30 minutes independently of the traffic load. The roads A and D are mountain roads and the travel time is estimated to about 10+x minutes where x is the traffic intensity in cars per minute (in one direction). During rush hours the total traffic between the cities in either direction s is about 20 cars per minute.

a) Assuming that every individual tries to optimize his/her own travel time, what will be the travel time during rush hours? Motivate your answer. Hint: consider if all individual decisions of drivers could eventually lead to some equilibrium state with constant traffic flows? (note that this is not a single optimization problem, but a more complex situation with many agents where each agent optimizes for itself)



Conditions:

B and C roads, time 30min independent of the traffic load.

A and D, 10+x min, in rush time traffic loading is cars/min

In the rush time, the total traffic between the cities in either direction s is about 20 cars per minute.

Variables:

The number of cars goes through B and D: x1 The number of cars goes through A and C: x2

Object function

For each car, the time spend to go trough B and D 30+10+x1 go through A and C 30+10+x2

The sum of the total number will be

The sum of the total number will be (30+10+x1)x1+(30+10+x2)x2

The problem is to find the minimum of the function (30+10+x1)x1+(30+10+x2)x2

Constraints

In a rush time: x1+x2=20 x1 and x2 >=0 x1 and x2 are integers.

Results

```
In[7]:= NMinimize[{(30+10+x1) x1+ (30+10+x2) x2, x1+x2 == 20, x1 \ge 0, x2 \ge 0, x1 \in Integers, x2 \in Integers}, {x1, x2}]

Out[7]:= {1 000., {x1 \to 10, x2 \to 10}}
```

The minimum total sum of the time is 1000 minutes and with 10 cars go through A and D and 10 cars go through B and C. Eventually, the equilibrium state is the number of person goes A and C equals to the number of person goes B and D.

b) In order to improve traffic flow it is decided to build a bridge over the river between the two small communities. The travel time over the bridge is about 1 minute independently of the traffic volumes we are considering. Again, assuming that every individual tries to optimize his/her own travel time, what will be the new travel time between the large cities? Motivate your answer, discuss the result and draw qualitative conclusions.

Conditions:

B and C roads, time 30min independent of the traffic load.

A and D, time 10+x min, x is the cars per minute

Go through the bridge 1min independent of the traffic load.

In the rush time, the total traffic between the cities in either direction s is about 20 cars per minute.

Variables:

The number of cars goes through B and D: x1 The number of cars goes through B and C: x2 The number of cars goes through A and C: x3 The number of cars goes through A and D: x4

Object function

For each car the time spend to go trough B and D 30+10+(x1+x4) go through A and C 30+10+(x3+x4) go through B and C 30+1+30 go through A and D 10+(x3+x4)+1+10+(x1+x4) The sum of the total number will be (30+10+(x1+x4))x1+(30+10+(x3+x4))x3+(61)x2+(10+(x3+x4)+1+10+(x1+x4))x4

The problem is to find the minimum of the function: (40+(x1+x4))x1+(40+(x3+x4))x3+61x2+(21+(x3+2x4+x1))x4

Constraints

In a rush time: x1+x2+x3+x4=20 x1, x2, x3, x4 >=0 x1,x2,x3 and x4 are integers

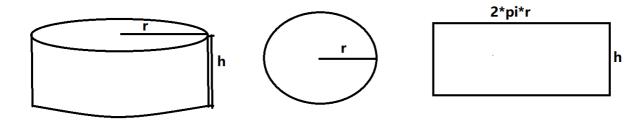
Results

The minimal sum of the time is 1000 minutes with x1 and x3 equal to 10, but x2, x4 equals 0. The bridge seems useless in this case.

```
 \begin{array}{l} & \text{In}[10] = \text{NMinimize}[\left\{\left(40 + (x1 + x4)\right) \times 1 + \left(40 + (x3 + x4)\right) \times 3 + 61 \times 2 + \left(31 + (x3 + 2 \times 4 + x1)\right) \times 4, \ x1 + x2 + x3 + x4 = 20, \ x1 \geq 0, \ x2 \geq 0, \ x3 \geq 0, \ x4 \geq 0, \ x1 \in \text{Integers}, \ x2 \in \text{Integers}, \ x3 \in \text{Integers}, \ x4 \in \text{Int
```

6.OPTIMAL SHAPE OF CAN

Take a careful look at how we modelled this problem in the lecture. Try Mathematica for this problem and find out what the best shape is! (Note that this is a non-linear optimization problem, which are usually harder to solve, but this is a very small one)



The shape of a can contains a circle and a rectangle.

and the volume of the cylinder is pi*r^2*h.

The surface of a can equals 2*pi*r*h+pi*r^2

The problem is to find the minimum of the can surface.

Object function:

2*pi*r*h+pi*r^2

Variable:

r and h

Constraints:

The volume of the cylinder is fixed, assume to be 1 pi*r^2*h=1

r and h >=0

Results:

```
In[9]:= FindMinimum[{2 Pirh + 2 Pir^2, Pir^2h == 1, r \ge 0, h \ge 0}, {r, h}]

Out[9]= {5.53581, {r \to 0.541926, h \to 1.08385}}
```

The minimal surface of a can is 5.54 with r 0.54 and h 1.08.

7.(EMERGENCY CARE PROBLEM)

The following problem is a so called facility location problem. A city wishes to make a long term study to decide where to best locate emergency care. The city has been partitioned into regions, and it has been decided that an emergency care site can

acceptably service regions of the city which are within a driving distance of 8 minutes. The goal is to choose a set of stations at minimum cost. There are seven regions to cover, and six potential sites have been identified. Distances in minutes between regions and potential sites:

Site #	1	2	3	4	5	6
Region 1	15	3	12	5	17	20
Region 2	12	9	13	16	3	4
Region 3	13	16	9	4	7	11
Region 4	3	7	6	22	5	18
Region 5	4	22	12	5	16	14
Region 6	8	10	5	16	13	5
Region 7	13	10	5	6	13	21

The cost for locating emergency care on the respective sites:

	Cost
Site 1	710 000
Site 2	610 000
Site 3	650 000
Site 4	910 000
Site 5	720 000
Site 6	570 000

a) Model this problem mathematically by defining variables, constraints and an objective function. To get started, you can simply begin to define some variables, write some equations and see what you get along the way. (It is best if you can make the constraints and the objective function linear, since then the problem becomes easier to solve mathematically. For links about linear programming see below. Note that in this step you are not solving the problem, just defining it. Hint: think about what I said in the lecture about how to define the variables.

Site 1 can connect to region 4, 5 and 6 because the distances are smaller than 8 minuter. So as to the rest of sites see bellowing

S1 (4,5,6)

S2 (1,4)

S3 (4,6,7)

S4 (1,3,5,7)

S5 (2,3,4)

S6 (2,6)

Assume the numbers of site1, site 2.. site 6 equal to x1, x2...x6.

```
The problem is to find the minimun of object function:
710000x1+610000x2+650000x3+910000x4+720000x5+570000x6
Variables:
site1, x1; site2, x2; site3, x3; site4, x4; site5, x5; site6,x6
Constraints
x1,x2,x3,x4,x5,x6 >= 0
The maximun sites' building must be smaller than 6:
0 < x1 + x2 + x3 + x4 + x5 + x6 < = 6
The region1 only accessible from site2 and site4 so that
1<=x2+x4<=2
same to the rest regions
region2:
1<=x5+x6<=2
region3:
1<=x4+x5<=2
region4:
1<=x1+x2+x3+x5<=4
region5
1 <= x1 + x4 <= 2
region6:
1<=x1+x3+x6<=3
All x1,x2,x3,x4,x5,x6 are intergers.
```

b) Now try to solve your model by using the Mathematica function NMinimize. Try to solve it as a plain linear programming problem with continuous variables (without using any special options of the NMinimize function or constraints to say that the variables are integer or binary - as we discussed in the introductory lecture). Describe any difficulties you run into. What conclusions can you draw from the solution you obtain? Then solve the original integer problem eg. by solving variations of the LP multiple times, or by using some integer option in Mathematica, and give the answer.

Without any special options of the NMinimin function or constraints for variables of integer or binary, I could get the minimal cost 1.67E6 units but with the numbers of sites in float type. It is not realistic to have 0.333 site located.

By using the integer option in Mathematica, the minimal cost of locating sites is 2.04E6 units with x1 (site1),x2 (site2) and x5 (site5) equal to 1 and x3, x4, x6 equal to 0. The cost is minimized by locating site1, site2 and site5.

```
In[10]:= NMinimize[ {710000 x1 + 610000 x2 + 650000 x3 + 910000 x4 + 720000 x5 + 570000 x6, 0 < x1 + x2 + x3 + x4 + x5 + x6 ≤ 6, 1 ≤ x2 + x4 ≤ 2, 1 ≤ x5 + x6 ≤ 2, 1 ≤ x4 + x5 ≤ 2, 1 ≤ x1 + x2 + x3 + x5 ≤ 4, 1 ≤ x1 + x4 ≤ 2, 1 ≤ x1 + x3 + x6 ≤ 3, x1 ≥ 0, x2 ≥ 0, x3 ≥ 0, x4 ≥ 0, x5 ≥ 0, x6 ≥ 0, x1 ∈ Integers, x2 ∈ Integers, x3 ∈ Integers, x4 ∈ Integers, x5 ∈ Integers, x6 ∈ Integers }, {x1, x2, x3, x4, x5, x6}]

Out[10]:= {2.04 x 10<sup>6</sup>, {x1 → 1, x2 → 1, x3 → 0, x4 → 0, x5 → 1, x6 → 0}}
```

c) Ask yourself if this is the only way to handle this problem? For example, in this problem we assumed that we should have a maximum number of minutes from each region of the city. Is this the only way to think about this? If you can, elaborate on any idea you might have. Note that while this problem only has a small number of variables and therefore can be solved by brute force combinatorial search, this would be useless for larger problems. For larger problems the more mathematical approach is much more powerful.

The shortest distance from each region or the traffic loading between each region, the maximum number of person is able to be treated.

8.(REASONING - PSYCHOLOGICAL TEST)

For each of the four cards below there is a letter on one side and a digit on the other.

F 8 U 3

For these cards it is also claimed that if there is a vowel on one side, there is an odd number on the other side. What is the least number of cards you need to turn to verify this, and which cards do you need to turn?

Problem:

To verify there is a vowel on one side and the other side number is an odd Constraints

a vowel -> an odd (Does not mean an odd -> a vowel), it is a sufficient but not necessary condition

Solution:

I need two times to verify this. The cards I need to turn is card U and card 8.

Reason

Card F is not a vowel, it doesn't matter if the other side is an odd number or not, it is not included in constraint.

Card 3 is an odd number, it doesn't matter if the other side is a vowel or not, it is not included the constraints.

Card U is a vowel, the other side must be check, if it is not odd, it will break the constraint. Card 8 is an even number, the other side must be check, if the other side is a vowel, it will break the constraint.

```
(finally...)
(MID-COURSE FEEDBACK)
```

The purpose of this question is to ensure a common understanding of what we are trying to do in this course, and to identify any possible problems. Your answers may influence our feedback and other actions during the rest of the course.

a) Please write what you think is the purpose of this course. If you like, you may also write a personal answer in terms of how you see the purpose of the course for you.

The course for me is to study how to think or plan my daily work mathematically. I am a problem-solution oriented person. I want to apply those mathematical methods which I studied in my daily life which help me be more logical and systematic.

- b) Does the course work well for you? If not, please explain! Yes, it works very well for me.
- c) Any other comments?

Some mathematical knowledge is lacked when solving the problems in modules. It might become better if I can be given some hints during the lecture on Monday.

d) What is your math background? The main distinction for us is "high school" or "university", but you are welcome to provide additional information if you wish. Please also give your main field of study in your BSc.

My math background is at the university level and I passed the mathematic 4 from Sweden before I took the course. I have 6 year- experience about data analysis by doing research at university. My background is theoretical chemistry. I am interested in being a data scientists now.

(finally...)
(SELF-CHECK)
Self-check passed!

Reflection

I spent 20 hours and tried my best to solve those problems in module 2. I went to supervision 2 times in a week.

The first task in module 4 is quite straightforward to me. The problem is to find out the relationship between income and the price of a chocolate bar. It can not directly be solved by looking at the data which is for quantity and price. But I could get the function for quantity, price and total income. The total income=quantity*price. By plotting the data, the relationship linked to a linear equation between price and quantity can be solved. by replacing the quantity using the resulting function, the relationship between income and price can be built. The maximal income can thus be solved when the derivative of the function equal to zero.

For the second task, the solution for problem a) is quite straightforward. I could find one reason for using the sum of square errors instead of the sum of the errors for each point. The negative and positive errors will not be canceled out using the sum of square errors. In the following-up lecture, I was taught the other reason is that the sum of square errors follows the convenient mathematical properties e.g. continuous differentiable.

In the third task, I solve the problem quite straightforward although I didn't know what the actual situation I need to figure out. The model is defined to find a minimum, the constraints

for the variables are also defined. By using the Mathematics program, the minimum is solved quite easily. In the follow-up lecture, I knew the actual situation to solve.

In the fourth task, I had experience for dynamic simulation calculation for protein folding. I used my previous experience to identify the global minimum and local minimum of the protein folding process.

In the fifth task, I was a bit confused by the units used in the problem. After attending the supervisor, I could understand the problem better. After that, I could solve the question by building a model assuming that all the drivers had made the best choice finally so that the equilibrium points will be located at the minimum time used under the rush traffic situation. Actually, the equilibrium situation is created by multiple individual decision in own favor. A+C=B+D, when each route gets half of the total traffic (30+(10+30)=50). With the bridge two decision movements (at the beginning and at the bridge). Choosing potentially the better alternative-common sense decision-does not lead to the best outcome. The bridge is independent of the constraints so it would not make any effect.

The sixth task, I could solve the problem quite straightforward because I had been given the hint in Monday's lecture. The problem is to find the lowest cost to make a can, which turns out the smallest amount of material to use. The problem becomes to find the smallest surface for a can. The problem and variables are defined. The volume depends on the volume of the product, so the constraints are also defined.

In the seventh task, in the beginning, it was very hard to find out the proper model to solve the questions. I didn't get the actual problem I need to solve. I listed all the possible combinations and then try calculate the total cost for those combinations. After a while, I find the problem is to find the lowest cost for building the sites. I can assume all those sites are possible to build and let the program to find out the optimal results. I could define the constraints by the actual situations.

In the eighth task, I was made some mistakes at the beginning without thinking so much. But after thinking for a while, I could solve the problem using efficient and necessary roles in mathematics to find out the exact constraints in the problem.

Summarize

In this module,

I learned how I could build a potential relationship based on a known relationship.

Furthermore, I learned the sum of square errors which can be used to evaluate how good the fitting is. Compared to sum of the errors, sum of square errors avoids canceling the errors in positive and negative values, and its convenient mathematical properties e.g. continuous differentiable, follows the convenient mathematical properties.

I learned to solve the problem to find out a minimal point:

1. identify the problem

- 2. identify the variables
- 3. build a mathematical model
- 4. find out the constraints among variables

I learned to use Nminimize function in Mathematics program.

In the last of this module, I learned the necessary and sufficient conditions which could help me to identify the constraints when solving a problem.