



YD :=

...\GY.xls

RD :=

...\GR.xls

Definition

Objective function

$$T := \begin{cases} \text{for } i \in 1.. \text{Vol11}_{0,1} \\ T_i \leftarrow T0_i - T0_{i-1} \\ T \\ a1 := 0.467 \end{cases}$$

$$Y(a2, aa, ab, ac, ad) := \begin{cases} \text{for } i \in 0.. \text{Vol11}_{0,1} \\ Y_i \leftarrow \sum_{i=0}^i \left[a1 \cdot aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + a2 \cdot ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \cdot \exp\left[-\sum_{i=0}^i \left[aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \cdot T_1 \right] \\ Y \end{cases}$$

You fooled me (and maybe yourself) by using "i" in different places for different things. And I was wrong when I said that Mathcad would handle it anyway.

You have to decide which of the following two interpretations is the one you had in mind:

$$Y1(a2, aa, ab, ac, ad) := \begin{cases} \text{for } n \in 0.. \text{Vol11}_{0,1} \\ Y_n \leftarrow \sum_{i=0}^n \left[\left[a1 \cdot aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + a2 \cdot ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \cdot \exp\left[-\sum_{k=0}^i \left[aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_k + 273)}\right] + ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_k + 273)}\right] \right] \cdot T_1 \right] \cdot T_1 \right] \\ Y \end{cases} \quad \text{note the upper limit "i" in the second sum}$$

or is it rather this one:

$$Y2(a2, aa, ab, ac, ad) := \begin{cases} \text{for } n \in 0.. \text{Vol11}_{0,1} \\ Y_n \leftarrow \sum_{i=0}^n \left[\left[a1 \cdot aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + a2 \cdot ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \cdot \exp\left[-\sum_{k=0}^n \left[aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_k + 273)}\right] + ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_k + 273)}\right] \right] \cdot T_1 \right] \cdot T_1 \right] \\ Y \end{cases} \quad \text{note the upper limit "n" in the second sum}$$

Both variants can be speeded up significantly:

$$Y1_{\text{speed}}(a2, aa, ab, ac, ad) := \begin{cases} \text{for } i \in 0.. \text{Vol11}_{0,1} \\ \text{Tmp}_i \leftarrow \exp\left[-T_1 \cdot \sum_{k=0}^i \left[aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_k + 273)}\right] + ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_k + 273)}\right] \right] \right] \\ \text{for } n \in 0.. \text{Vol11}_{0,1} \\ Y_n \leftarrow T_1 \cdot \sum_{i=0}^n \left[\left[a1 \cdot aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + a2 \cdot ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \cdot \text{Tmp}_i \right] \\ Y \end{cases}$$

$$Y2_{\text{speed}}(a2, aa, ab, ac, ad) := \begin{cases} \text{for } n \in 0.. \text{Vol11}_{0,1} \\ \text{Tmp} \leftarrow \exp\left[-\sum_{k=0}^n \left[aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_k + 273)}\right] + ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_k + 273)}\right] \right] \cdot T_1 \right] \\ Y_n \leftarrow \text{Tmp} \cdot T_1 \cdot \sum_{i=0}^n \left[\left[a1 \cdot aa \cdot \exp\left[\frac{-ac}{R \cdot (TT1_i + 273)}\right] + a2 \cdot ab \cdot \exp\left[\frac{-ad}{R \cdot (TT1_i + 273)}\right] \right] \right] \\ Y \end{cases}$$

OK, before going any further lets check whats different and lets introduce a timer to see if the "speed" routines do what they are supposed to do (the caclulation take a few seconds/minutes, be patient):

$$\text{timer}(f) := \begin{cases} t1 \leftarrow \text{time}(0) \\ R \leftarrow f(0.86, 10^5, 10^5, 76800, 14000) \\ \left(\begin{array}{c} \text{time}(0) - t1 \\ R \end{array} \right) \end{cases}$$

$$\begin{pmatrix} \text{time_Y} \\ \text{YY} \end{pmatrix} := \text{timer}(Y) \quad \begin{pmatrix} \text{time_Y1} \\ \text{YY1} \end{pmatrix} := \text{timer}(Y1) \quad \begin{pmatrix} \text{time_Y2} \\ \text{YY2} \end{pmatrix} := \text{timer}(Y2) \quad \begin{pmatrix} \text{time_Y1}_{\text{sp}} \\ \text{YY1}_{\text{sp}} \end{pmatrix} := \text{timer}(Y1_{\text{speed}}) \quad \begin{pmatrix} \text{time_Y2}_{\text{sp}} \\ \text{YY2}_{\text{sp}} \end{pmatrix} := \text{timer}(Y2_{\text{speed}})$$

$$\text{time_Y} \cdot \text{s} = 11.549 \text{ s} \quad \text{time_Y1} \cdot \text{s} = 11.755 \text{ s} \quad \text{time_Y2} \cdot \text{s} = 22.861 \text{ s} \quad \text{time_Y1}_{\text{sp}} \cdot \text{s} = 0.158 \text{ s} \quad \text{time_Y2}_{\text{sp}} \cdot \text{s} = 0.14 \text{ s}$$

So I guess we can speak about a significant improvement by both "speed" variants

$$|\text{YY} - \text{YY1}| = 0 \quad \left| \text{YY1} - \text{YY1}_{\text{sp}} \right| = 7.699 \times 10^{-15} \quad \text{The shown deviation is within the numerical tolerance. We can probably say that your original routine Y and my modifications Y1 and Y1}_{\text{speed}} \text{ yield the very same result.}$$

$$|\text{YY} - \text{YY2}| = 18.997 \quad \left| \text{YY2} - \text{YY2}_{\text{sp}} \right| = 0 \quad \text{So the second interpretation of your expression with the many equal indices "i" differs from your original but I have no idea which interpretation is the correct one for your task}$$

Anyway, Y2 and Y2}_{\text{speed}} \text{ yield the very same result.}

Put any of the two speed-functions (whichever you think is the correct one) in the definition of OF and see if the solve block yields a result in reasonable time now.

At least OF calculates now approx. 50000 times faster than in your original sheet ;-)

$$\text{OF1}(a2, aa, ab, ac, ad) := \begin{cases} \text{YY} \leftarrow 100 Y1_{\text{speed}}(a2, aa, ab, ac, ad) \\ \sum_{i=0}^{\text{Vol1}1_{0,1}} (Y_{\text{exp}_i} - \text{YY}_i)^2 \end{cases} \quad \text{Just a test:} \quad \text{timer}(\text{OF1}) = \begin{pmatrix} 0.155 \\ 1.981 \times 10^6 \end{pmatrix}$$

$$aa := 10^5 \quad ab := 10^5 \quad ac := 76800 \quad ad := 140000 \quad a2 := 0.86$$

$$t1 := \text{time}(0)$$

Given

$$10^3 \leq aa \leq 10^6 \quad 10^5 \leq ab \leq 10^8 \quad 70000 \leq ac \leq 120000$$

$$120000 \leq ad \leq 170000 \quad a1 \leq a2 \leq 1$$

$$\begin{pmatrix} a2 \\ aa \\ ab \\ ac \\ ad \end{pmatrix} := \text{Minimize}(\text{OF1}, a2, aa, ab, ac, ad) = \begin{pmatrix} 0.531 \\ 1.672 \times 10^5 \\ 1.037 \times 10^5 \\ 7 \times 10^4 \\ 1.7 \times 10^5 \end{pmatrix}$$

$$(\text{time}(0) - t1) \text{s} = 1.372 \cdot \text{min} \quad \text{Time it took for the solve block to finish}$$

Check if the constraints are all OK:

$$10^3 \leq aa \leq 10^6 = 1 \quad 10^5 \leq ab \leq 10^8 = 1 \quad 70000 \leq ac \leq 120000 = 1$$

$$120000 \leq ad \leq 170000 = 1 \quad a1 \leq a2 \leq 1 = 1$$

$$\text{OF1}(a2, aa, ab, ac, ad) = 1.622 \times 10^4$$

$$\begin{pmatrix} 0.531 \\ 1.672 \times 10^5 \\ 1.037 \times 10^5 \\ 7 \times 10^4 \\ 1.7 \times 10^5 \end{pmatrix}$$

Now the same with variant 2:

$$\text{OF2}(a2, aa, ab, ac, ad) := \begin{cases} YY \leftarrow 100 Y2_{\text{speed}}(a2, aa, ab, ac, ad) \\ \sum_{i=0}^{\text{Vol11}_{0,1}} (Y_{\text{exp}_i} - YY_i)^2 \end{cases} \quad \text{timer}(\text{OF2}) = \begin{pmatrix} 0.135 \\ 4.955 \times 10^5 \end{pmatrix}$$

$$aa := 10^5 \quad ab := 10^5 \quad ac := 76800 \quad ad := 140000 \quad a2 := 0.86$$

t1 := time(0)

Given

$$10^3 \leq aa \leq 10^6 \quad 10^5 \leq ab \leq 10^8 \quad 70000 \leq ac \leq 120000$$

$$120000 \leq ad \leq 170000 \quad a1 \leq a2 \leq 1$$

$$\begin{pmatrix} a2 \\ aa \\ ab \\ ac \\ ad \end{pmatrix} := \text{Minimize}(\text{OF2}, a2, aa, ab, ac, ad) = \begin{pmatrix} 1 \\ 1000 \\ 1.557 \times 10^7 \\ 1.2 \times 10^5 \\ 1.2 \times 10^5 \end{pmatrix}$$

(time(0) - t1)s = 3.099·min *Time it took for the solve block to finish*

Check if the constraints are all OK:

$$10^3 \leq aa \leq 10^6 = 0 \quad 10^5 \leq ab \leq 10^8 = 1 \quad 70000 \leq ac \leq 120000 = 1$$

$$120000 \leq ad \leq 170000 = 1 \quad a1 \leq a2 \leq 1 = 0 \quad \text{So we see that two constraints were not respected!}$$

$$\text{OF2}(a2, aa, ab, ac, ad) = 3.014 \times 10^4$$

▣ Objective function

Time111 := $\left\{ \begin{array}{l} \text{for } i \in 0.. \text{Voll1}_{0,1} - \text{Voll1}_{0,1} \\ \text{Time111}_i \leftarrow \text{Time11}_{i+\text{Voll1}_{0,1}} \\ \text{Time111} \end{array} \right.$