Lecture 21 - Nonlinear Equations II

- Prayer/Spiritual Thought
- Announcements

Outline

1. Solve blocks with parameters
2. Best practices with solve blocks
3. Debugging solve blocks

1. Solve blocks with parameters

A. Explanation

- Sometimes you want to solve a nonlinear equation multiple times while varying a parameter.
- We can do this by making a solve block where:

    1. We leave the parameter *unspecified*
    2. We define a function using **find**

- This is best explained with an example:

B. Example

Suppose we are trying to find the temperature of a saturated vapor using a vapor pressure correlation:

$$P_{sat}(T) := \exp\left(73.649 - 7258.2 \cdot \left(\frac{T}{K}\right)^{-1} - 7.3037 \cdot \ln\left(\frac{T}{K}\right) + 4.1653 \cdot 10^{-6} \cdot \left(\frac{T}{K}\right)^{2}\right) \cdot Pa$$

(Old) Typical Solve block

$P := 2299 \cdot kPa$ This is a single pressure where we want to find the temperature.

Guess Values

$T_{guess} := 500\ K$

Constraints

$P_{sat}(T_{guess}) = P$

Solver

$T_1 := \mathrm{Find}(T_{guess}) = 492.78\ K$

(New) Now treat pressure as a parameter. Solve
for MANY values of T as a function of P.

Guess Values / Constraints / Solver

$T_{guess} := 500\ K$

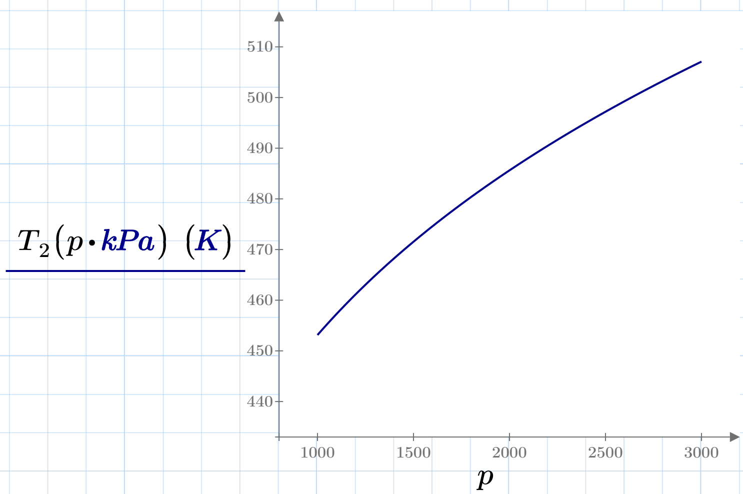
$P_{sat}(T_{guess}) = P_{new}$ <-- We have not defined Pnew!

$T_2(P_{new}) := \mathbf{Find}(T_{guess})$ <-- T2 is a *function* of Pnew

$T_2(2299\ kPa) = 492.78\ K$ <-- This is the same answer!

$T_2(3000\ kPa) = 507.088\ K$ <-- We can easily solve for this temp
without a new solve block!

We can even make a plot with this new function.



Tip:

- To make a plot with a function that has units, you need to put units inside the function argument like this example.

2. Best practices with solve blocks

A. Explanation

- Like solver in Excel, solve blocks in Mathcad are quite powerful. However, solve blocks are not all powerful, and they can fail to give an answer. There is a lot of algorithmic complexity happening underneath the hood.
- This means there are some **best practices** (rules you should generally follow unless you have a reason not to) that help you get an answer when using solve blocks.

B. List of best practices

1. Wherever possible, reduce the number of equations and variables.
2. Arrange equations to avoid
    - fractional powers (e.g. square roots)
    - logs
    - poles (infinite discontinuities)
3. Make a smart guess. Your guess should:
    - Obey the constraints of the problem
    - Make physical sense
    - Be the right sign
    - Be guided by a plot

- These best practices help reduce the dimensionality of the problem and make it easier for your guess to be close enough to converge to an answer.

C. Examples

(i) Reducing equations

Remember our vapor/liquid equilibrium problem from last time:

$$y_1 \cdot P = x_1 \cdot P_{sat_1} \qquad y_2 \cdot P = x_2 \cdot P_{sat_2}$$

$$y_1 + y_2 = 1 \qquad x_1 + x_2 = 1$$

$$ln\left(P_{sat_i}\right) = A_i - \frac{B_i}{T + C_i}$$

Given quantities

$P := 120 \qquad y_1 := 0.33$

$A_1 := 13.7819 \qquad B_1 := 2726.81 \qquad C_1 := 217.572$

$A_2 := 13.9320 \qquad B_2 := 3056.96 \qquad C_2 := 217.625$

(Bad example) -- Using too many unnecessary equations

Guess Values

$x_1 := 0.4$ $x_2 := 0.5$ $y_2 := 0.1$

$T := 50$ $P_{sat\_1} := 100$ $P_{sat\_2} := 100$

6 equations and 6 unknowns! That is a lot of places for guesses to go wrong.

Constraints

$y_1 \cdot P = x_1 \cdot P_{sat\_1}$ $x_1 + x_2 = 1$

$y_2 \cdot P = x_2 \cdot P_{sat\_2}$ $y_1 + y_2 = 1$

$$ln\left(P_{sat\_1}\right) = A_1 - \frac{B_1}{T + C_1}$$

$$ln\left(P_{sat\_2}\right) = A_2 - \frac{B_2}{T + C_2}$$

Solver

$$\text{Find}\left(x_1, x_2, y_2, P_{sat\_1}, P_{sat\_2}, T\right) = \begin{bmatrix} 0.173 \\ 0.827 \\ 0.67 \\ 229.396 \\ 97.175 \\ 109.131 \end{bmatrix}$$

Luckily this one still converges to the right answer.

(Good example) -- Eliminate unnecessary intermediates

Guess Values

$x_1 := 0.5$ $T := 300$

<-- Now I only have 2 equations and 2 unknowns.

Constraints

$$y_1 \cdot P = x_1 \cdot exp\left(A_1 - \frac{B_1}{T + C_1}\right)$$

$$\left(1 - y_1\right) \cdot P = \left(1 - x_1\right) \cdot exp\left(A_2 - \frac{B_2}{T + C_2}\right)$$

Solver

$$\text{Find}\left(x_1, T\right) = \begin{bmatrix} 0.173 \\ 109.131 \end{bmatrix}$$

(ii) Bad guesses

Consider the liquid-liquid equilibrium between a polymer and a solvent

$$\mu_1(\phi_a) = \mu_1(\phi_b)$$

$$\mu_2(\phi_a) = \mu_2(\phi_b)$$

$$\mu_1 = ln(\phi) + (1-\phi) \cdot \left(1 - \frac{1}{N}\right) + \chi \cdot (1-\phi)^2$$

$$\mu_2 = \frac{1}{N} ln(1-\phi) + \phi \cdot \left(\frac{1}{N} - 1\right) + \chi \cdot \phi^2$$

where phi_a, phi_b are the volume fractions of the solvent in phase a and b respectively. N and Chi are parameters which describe the polymer size and interaction between polymer and solvent. Assume $N = 10$ and $\chi = 2.5$.

$N := 10$ $\quad\quad$ $\chi := 2.5$

$$\mu_1(\phi) := \ln(\phi) + (1-\phi) \cdot \left(1 - \frac{1}{N}\right) + \chi \cdot (1-\phi)^2$$

$$\mu_2(\phi) := \frac{1}{N} \ln(1-\phi) + \phi \cdot \left(\frac{1}{N} - 1\right) + \chi \cdot \phi^2$$

The logs are unavoidable here. This makes this problem hard.

Guess Values

$\phi_a := 0.1$ $\quad\quad$ $\phi_b := 0.999$

Constraints

$\mu_1(\phi_a) = \mu_1(\phi_b)$ $\quad\quad$ $\mu_2(\phi_a) = \mu_2(\phi_b)$

Solver

$$\textbf{Find}(\phi_a, \phi_b) = \begin{bmatrix} 0.04275238 \\ 0.99999992 \end{bmatrix}$$

<-- Try different guesses:
* negative
* out of physcial bounds (0, 1)
* A guess where phi_a is close to 0 and phi_b is very close to 1 will work.

<-- These should be different numbers. If they are the same, it is not the right answer.

3. Debugging solve blocks

A. Explanation

- It can be hard to find syntax errors or other mistakes inside solve blocks.
- Like programming, good debugging skills are won with practice and experience, but some general tips can also help.

B. List of debugging techniques

1. Check to make sure that all functions defined before the solve block work properly
2. Copy the LHS and RHS of the equations in the solve block to check:
    - Calculation
    - Units
    - Order of magnitude
3. Don't over/under specify the problem. In other words the number of guesses should equal the number of equations which should also equal the number of variables in the find statement.
4. Ensure that each solve block has:
    - Guesses
    - Equations
    - Find
5. Double check your variables. Make sure the guesses, equations, and find are all written with the same variables.

C. Examples

Debug the following solve block

$\rho := 55.19 \frac{kg}{m^3}$ $\mu := 0.00087645 \cdot Pa \cdot s$ $\varepsilon := 1.524 \cdot 10^{-3} \cdot mm$

$D := 1.91 \cdot cm$ $\Delta P := -70 \cdot kPa$ $Len := 20 \cdot m$

Guess Values

$v_g := 2 \frac{m}{s}$ $f_g := 10^{-3}$

Constraints

$$\frac{\Delta P}{\rho} = -f_g \cdot \frac{Len}{D} \cdot \frac{v_g^2}{2} \qquad \frac{1}{\sqrt{f_g}} = -2 \cdot \log\left(\frac{\varepsilon \cdot D}{3.7} + \frac{2.51}{\frac{\rho \cdot D \cdot v_g}{\mu} \cdot \sqrt{f_g}}\right)$$

Solver

$$\begin{bmatrix} vv \\ ff \end{bmatrix} := \mathbf{Find}\left(v_g, \mathrm{f_g}\right) = ?$$

(for reference, the fixed solve block)

Guess Values

$$v_g := 2\ \frac{m}{s} \qquad f_g := 10^{-3}$$

Constraints

$$\frac{\Delta P}{\rho} = -f_g \cdot \frac{Len}{D} \cdot \frac{{v_g}^2}{2} \qquad \frac{1}{\sqrt{f_g}} = -2 \cdot log\left(\frac{\varepsilon}{3.7 \cdot D} + \frac{2.51}{\frac{\rho \cdot D \cdot v_g}{\mu} \cdot \sqrt{f_g}}\right)$$

Solver

$$\begin{bmatrix} vv \\ ff \end{bmatrix} := \textbf{Find}\left(v_g, f_g\right) = \begin{bmatrix} 8.921\ \frac{m}{s} \\ 0.03 \end{bmatrix}$$