

Indian Institute of Technology Roorkee

**CHN-323**

# **Computer Applications in Chemical Engineering**

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# Example 1

Consider the data set shown in Table. The data comes from the domain of heat transfer in pipes.

- The input variables (x) are: Re, Pr, Mu
- The response variable y is Nu.
- It is desired to fit a model of the form

$$Nu = aRe^bPr^cMu^d$$

- Determine the parameters of the model (i.e. a, b, c and d).
- Make a plot of the model fit versus the experimental data and label the graph suitably.

Sample No.	Re	Pr	Mu	Nu
1	49000	2.3	0.947	277
2	68600	2.28	0.954	348
3	84800	2.27	0.959	421
4	34200	2.32	0.943	223
5	22900	2.36	0.936	177
6	1321	246	0.592	114.8
7	931	247	0.583	95.9
8	518	251	0.579	68.3
9	346	273	0.29	49.1
10	122.9	1518	0.294	56
11	54	1590	0.279	39.9
12	84.6	1521	0.267	47
13	1249	107.4	0.724	94.2
14	1021	186	0.612	99.9
15	465	414	0.512	83.1
16	54.8	1302	0.273	35.9

# Example 2

- The following model is proposed to capture the trend in adjacent data

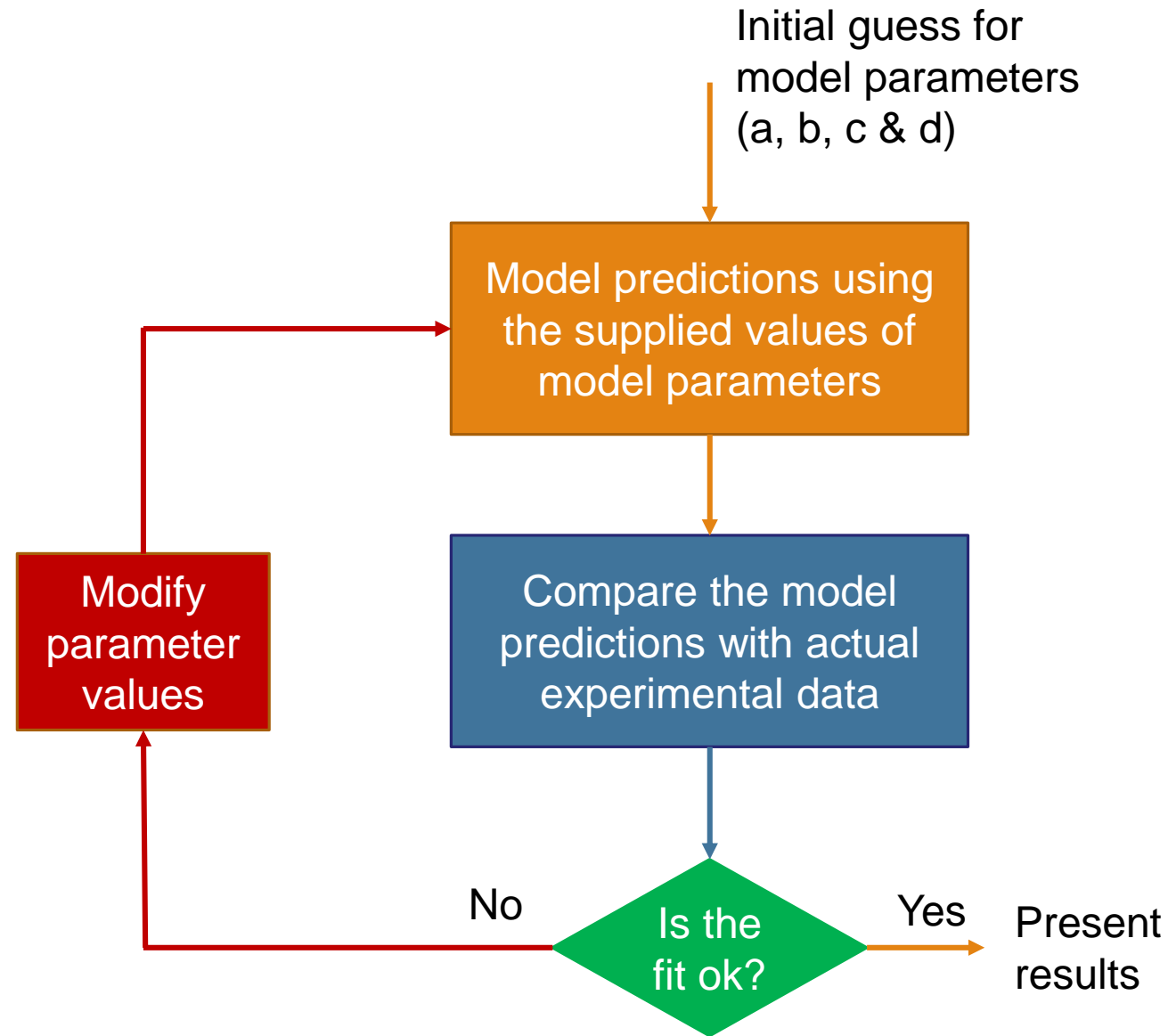
$$y = k_1 e^{k_2 x} + k_3$$

where  $k_1$ ,  $k_2$  and  $k_3$  are model parameters

- Determine the model parameters
- Make a plot of the model fit versus the experimental data and label the graph suitably.

x	y
0	12
1	11.0937
2	10.3516
3	9.7441
4	9.2466
5	8.8394
6	8.506
7	8.233
8	8.0095
9	7.8265
10	7.6767

# Idea



# How to modify the parameter values?

- Randomly??
- Minimize the error using suitable optimization algorithms
- Error ??

# Error

- Residual error for  $i^{\text{th}}$  sample

$$e_i = y_{exp} - y_{mod}$$

where  $y$  is the response variable being predicted.

- Mean absolute error (MAE)

$$MAE = \frac{\sum_{i=1}^n |e_i|}{n}$$

where  $n$  is the total number of data samples

- Mean squared error (MSE)

$$MSE = \frac{\sum_{i=1}^n (e_i)^2}{n}$$

- Root mean squared error (RMSE)

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (e_i)^2}{n}}$$

# How to modify the parameter values?

- Randomly??
- Minimize the error using suitable optimization algorithms
- Error ??
- Minimize the error with respect to the model parameters

# How to modify the parameter values?

➤  $RMSE = \sqrt{\frac{\sum_{i=1}^n (e_i)^2}{n}} = \sqrt{\frac{\sum_{i=1}^n (y_{exp} - y_{mod})^2}{n}}$

➤ From the given model expression, we know that

$$y_{mod} = k_1 e^{k_2 x} + k_3$$

➤ If we substitute this in above RMSE expression, we can say that

$$RMSE = f(k_1, k_2, k_3)$$

➤ We have to minimize the above function wrt  $k_1$ ,  $k_2$ , and  $k_3$