Empirical Models

- These models are developed from experimental data via “curve fitting”.
- These models are not valid outside the range of experimental data used to develop them.
- The model parameters may not have any physical significance.

Fitting Models by Least Squares

1. Assume a form of the model with *unknown* coefficients.

2. Estimate model parameters that *minimize* the sum of the sqare of the error between experimental data and model prediction.

This parameter estimation problem can be posed as a problem of function minimization.

Linear Least Squares:

Suppose a variable y is a *linear* function of the variables x_1, x_2, ..., x_p. Thus:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + ... + \beta_p x_p \tag{1}$$

Suppose we measure y, x_1,x_2, ..., x_p at n different points where $n > p$ (usually $n >> p$) and have a table of the following form:

i	x_{1i}	x_{2i}	x_{3i}	.	.	x_{pi}	Y_i
1	.	.	.	.	.	.	
2	.	.	.	.	.	.	
3	.	.	.	.	.	.	
.	.	.	.	.	.	.	
.	.	.	.	.	.	.	
n	.	.	.	.	.	.	

The objective is to find parameters β_0, β_1, ..., β_p such that the sum of squares of the error between the experimental data Y_i and the model prediction given by equation (1) is *minimized*.

This can be posed as the following minimization problem:

$$min\ e = \sum_{i=1}^{n}(Y_i - y_i)^2 \tag{2}$$

where Y_i is the experimental data value of the i^{th} data point and y_i is the corresponding model prediction obtained by substituting x_i in equation 1.

This is equivalent to:

$$min\ e = \sum_{i=1}^{n}(Y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + ... + \beta_p x_{pi}))^2 \quad (3)$$

The necessary conditions of optimality are:

$$
\begin{aligned}
\frac{\partial e}{\partial \beta_0} &= 0 \\
\frac{\partial e}{\partial \beta_1} &= 0 \\
\frac{\partial e}{\partial \beta_2} &= 0 \\
&\cdot \\
&\cdot \\
\frac{\partial e}{\partial \beta_p} &= 0
\end{aligned}
\tag{4}
$$

$$\begin{aligned}
\frac{\partial e}{\partial \beta_0} &= \frac{\partial}{\partial \beta_0}(\sum_{i=1}^{n}(Y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + ... + \beta_p x_{pi}))^2 \\
&= 2(\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - ... - \beta_p x_{pi}))(-1)
\end{aligned} \tag{5}$$

Similarly:

$$\begin{aligned}
\frac{\partial e}{\partial \beta_1} &= \frac{\partial}{\partial \beta_1}(\sum_{i=1}^{n}(Y_i - (\beta_0 + \beta_1 x_{1i} + \beta_2 x_{2i} + ... + \beta_p x_{pi})^2 \\
&= 2(\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 x_{1i} - \beta_2 x_{2i} - ... - \beta_p x_{pi})(-x_{1i})
\end{aligned} \tag{6}$$

In this way, $p + 1$ necessary conditions can be written.

The necessary conditions of optimality simplify to the following $p+1$ equations in $p+1$ variables:

$$
\begin{aligned}
\beta_0 \sum 1 + \beta_1 \sum x_{1i} + \beta_2 \sum x_{2i} + ... + \beta_p \sum x_{pi} &= \sum Y_i \\
\beta_0 \sum x_{1i} + \beta_1 \sum x_{1i}x_{1i} + \beta_2 \sum x_{2i}x_{1i} + ... + \beta_p \sum x_{pi}x_{1i} &= \sum Y_i x_{1i} \\
\beta_0 \sum x_{2i} + \beta_1 \sum x_{1i}x_{2i} + \beta_2 \sum x_{2i}x_{2i} + ... + \beta_p \sum x_{pi}x_{2i} &= \sum Y_i x_{2i} \\
&\cdot \\
&\cdot \\
\beta_0 \sum x_{pi} + \beta_1 \sum x_{1i}x_{pi} + \beta_2 \sum x_{2i}x_{pi} + ... + \beta_p \sum x_{pi}x_{pi} &= \sum Y_i x_{pi}
\end{aligned} \tag{7}
$$

where $\sum$ implies $\displaystyle\sum_{i=1}^{n}$.

Procedure for calculating β_is

1. Tabulate x_{1i}, x_{2i}, ... x_{pi}, Y_i.
2. Compute the terms $x_{1i}x_{1i}$, $x_{1i}x_{2i}$, ..., $x_{pi}x_{pi}$, Y_ix_{1i}, Y_ix_{2i}, ..., Y_ix_{pi} and tabulate these values.
3. Add the columns of this table to compute the values of all the $\sum$ given in eq. (7) in the previous slide.
4. Substitute the values of all the $\sum$ in eq. (7).
5. There are $p+1$ equations in $p+1$ variables.
6. Solve these $p+1$ equations via Gaussian elimination (or Gauss Jordon or Successive Over-relaxation, ...) for β_0, β_1, ..., β_p.

Example 1

The cost of fabricating a heat exchanger can be *empirically* expressed as follows:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 \tag{8}$$

where

y	$=$	Cost of fabrication
x_1	$=$	Number of tubes
x_2	$=$	Shell Surface Area

Estimate the values of the constants β_0, β_1 and β_2 from the following data:

x_1	x_2	Y ($)
120	550	310
130	600	300
108	520	275
110	420	250
84	400	220
90	300	200
80	230	190
55	120	150
64	190	140
50	100	100