공정 모형 및 해석
최소 자승법

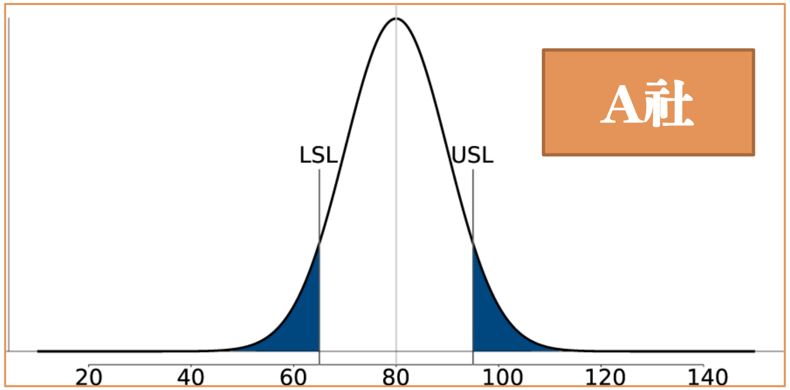
Jay Liu

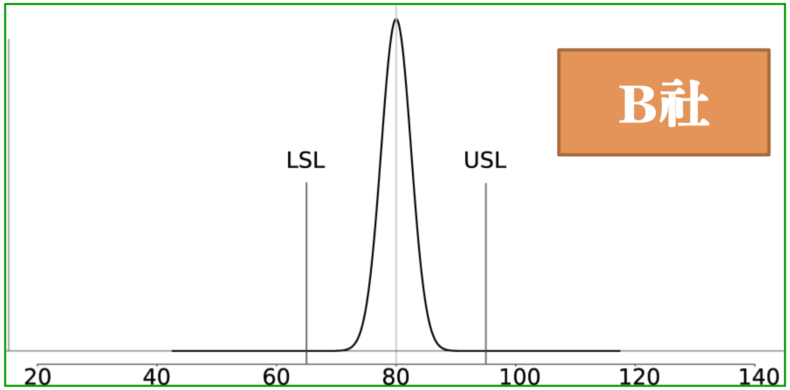
Dept. Chemical Engineering

PKNU

[FYI]Process capability (공정능력)

- Suppose you need to choose a raw material supplier among company A and company B. You received a database containing quality of a raw material from each company and plotted them with spec. limits (LSL and USL) that you product requests. Which one would you choose?





- How to quantify this capability?
- Which statistics are useful in describing this capability?

[FYI]Process capability (Cont.)

- C_p (or PCR, process capability ratio)

$$C_P = \frac{USL - LSL}{6\sigma}$$

- C_{pk} (or PCR_k) for one-sided limit

μ and σ: calculated from data

$$C_{pk} = \min\left(\frac{USL - \mu}{3\sigma}, \frac{\mu - LSL}{3\sigma}\right)$$

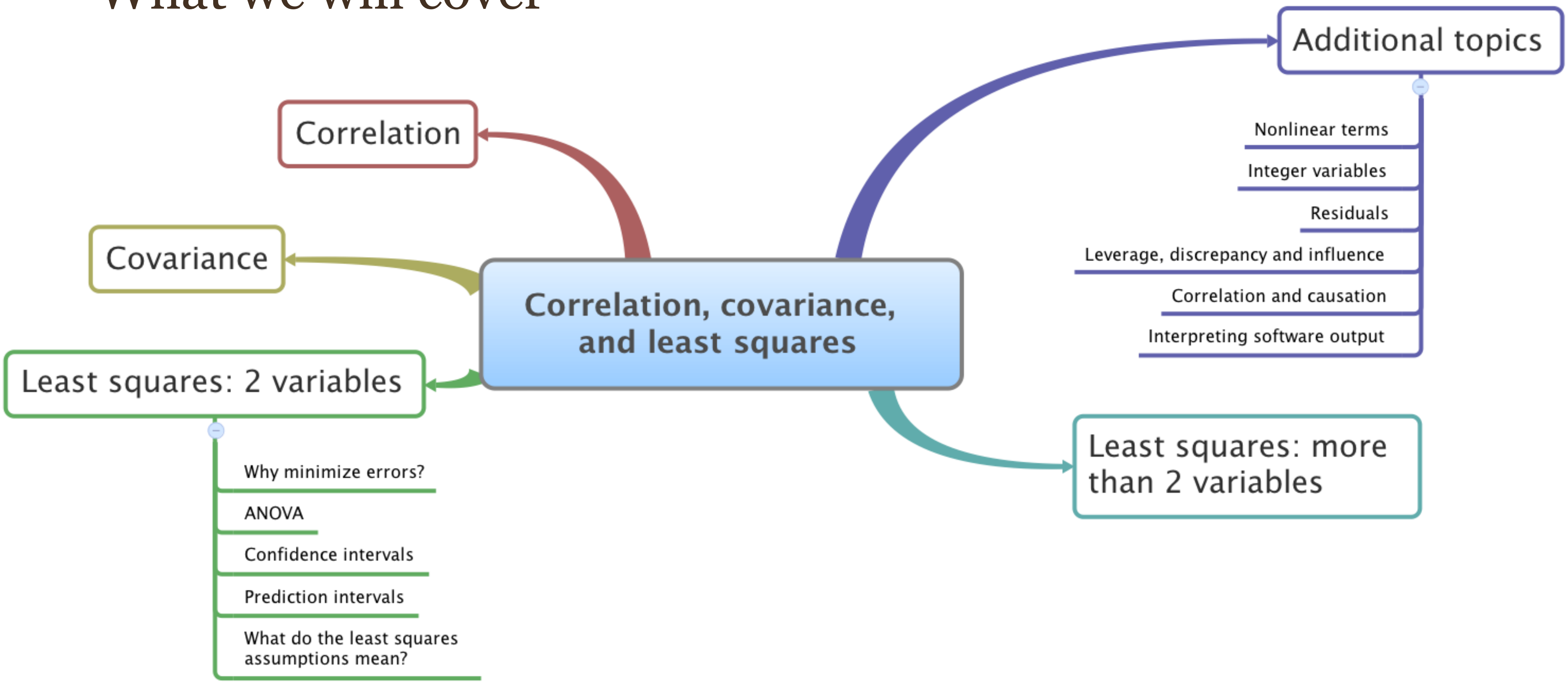
- In general, C_p (or C_{pk}) = 1.33 is minimum requirement

※Stat > quality tools > capability analysis

※Note: Cpk and Cp are only useful for a process which is stable

Least squares regression (최소자승회귀법)

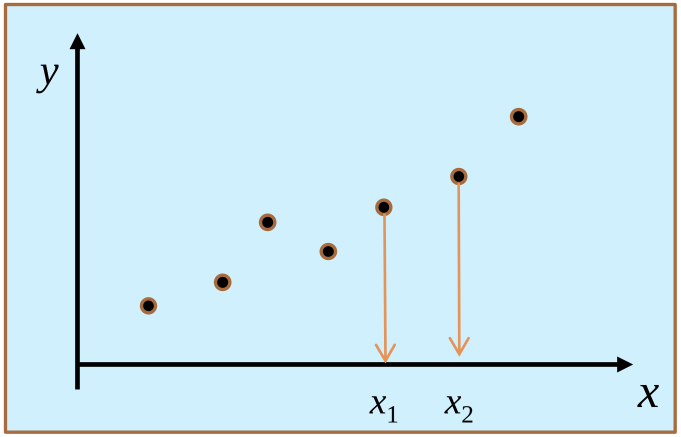
- What we will cover



Box, G.E.P., Use and abuse of regression, *Technometrics*, 8 (4), 625-629, 1966

[FYI]Least squares vs. interpolation

- Given the data, there are two choices when we want to know the value of y at $x = (x_1 + x_2)/2$



x	y
…	…
…	…
x_1	y1
x_2	y_2
…	…

  - least squares? or interpolation?
- Interpolation is recommended when data are subject to negligible experimental error (or noise)
  - Ex. In using steam tables
- Otherwise, least squares is recommended.

Least squares - usage examples (사용 예)

- Quantify relationship between 2 variables (or 2 sets of variables):
  - Manager: How does yield from the lactic acid batch fermentation relate to the purity of sucrose?
  - Engineer: The yield can be predicted from sucrose purity with an error of plus/minus 8%
  - Manager: And how about the relationship between yield and glucose purity?
  - Engineer: Over the range of our historical data, there is no discernible relationship.

Least squares - usage examples

- Two general applications
  - Predictive modeling – usually when an exact model form is unknown.
    - Modeling data trends in order to predict future y values
  - Simulation – usually when parameters in the model are unknown.
    - Getting parameter values in the known model form (e.g., calculate activation energy from reaction data)
- Terminology (용어)
  - y : response variables, output variables, dependent variables,
  - x : input variables, regressor variables, independent variables

Review: covariance (공분산)

- Consider measurements from a gas cylinder: temperature (K) and pressure (kPa).
- Ideal gas law applies under moderate condition: pV = nRT
  - Fixed volume, $V = 20 \times 10^{-3} m^3 = 20$ L
  - Moles of gas, n = 14.1 mols of chlorine gas, (1 kg gas)
  - Gas constant, R = 8.314 J/(mol.K)
- Simplify the ideal gas law to: $p = \beta_1 T$, where

$$\beta_1 = \frac{nR}{V}$$

Review: covariance (Cont.)

	Cylinder temperature (K)	Cylinder pressure (kPa)	Room humidity (%)
	273	1600	42
	285	1670	48
	297	1730	45
	309	1830	49
	321	1880	41
	333	1920	46
	345	2000	48
	357	2100	48
	369	2170	45
	381	2200	49
Mean	327	1910	46.1
Variance	1320	43267	8.1

Review: covariance (Cont.)

- Formal definition:

$$\text{cov}(x,y) = E\{(x-\bar{x})(y-\bar{y})\} \quad \text{where } E(z) = \bar{z}$$

1. Calculate deviation variables: $T-\bar{T}$ and $p-\bar{p}$
   - Subtracting off mean centers the vector at zero.
2. Multiply the centered values: $(T-\bar{T})(p-\bar{p})$
   - 16740 10080 5400 1440 180 60 1620 5700 10920 15660
3. Calculate the expected value (mean): 6780
4. Covariance has units: [K.kPa]

c.f) Covariance between temperature and humidity is 202

※ Covariance with itself is the variance:

$$\text{cov}(x,x) = V(x) = E\{(x-\bar{x})(x-\bar{x})\}$$

Review: correlation (상관관계)

Q: Which one (pressure and humidity) has stronger relationship with temperature?

- Covariance depends on units: e.g. different covariance for grams vs kilograms
- Correlation removes the scaling effect:

$$corr(x,y) = \frac{\text{cov}(x,y)}{\sigma_x \sigma_y} = \frac{E\left\{\left(x-\bar{x}\right)\left(y-\bar{y}\right)\right\}}{\sigma_x \sigma_y}$$

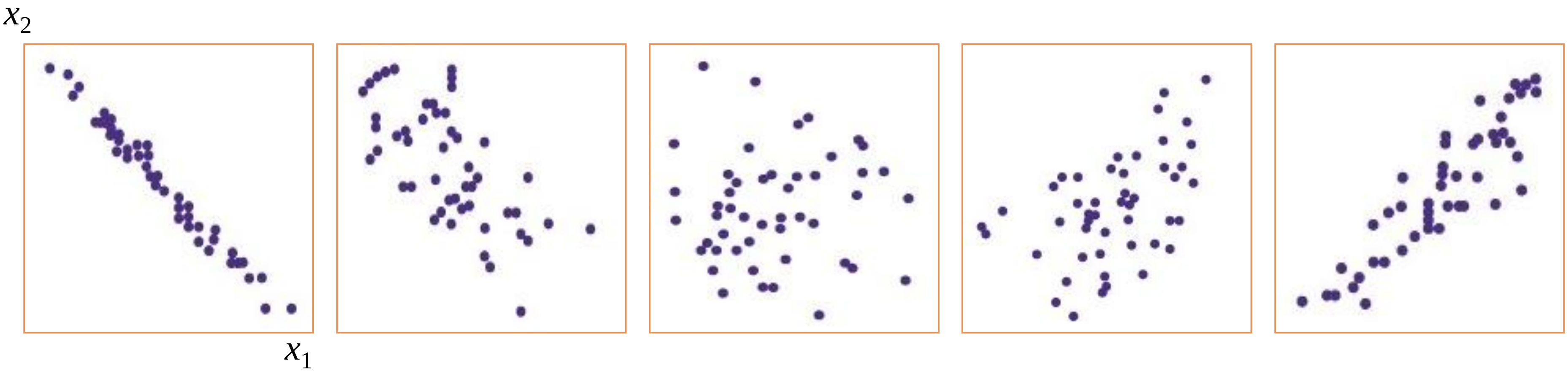
- Divides by the units of x and y: dimensionless result

$$-1 \le corr(x,y) = \rho_{xy} \le 1$$

- Gas cylinder example:
  - corr(temperature, pressure) = 0.997
  - corr(temperature, humidity) = 0.380

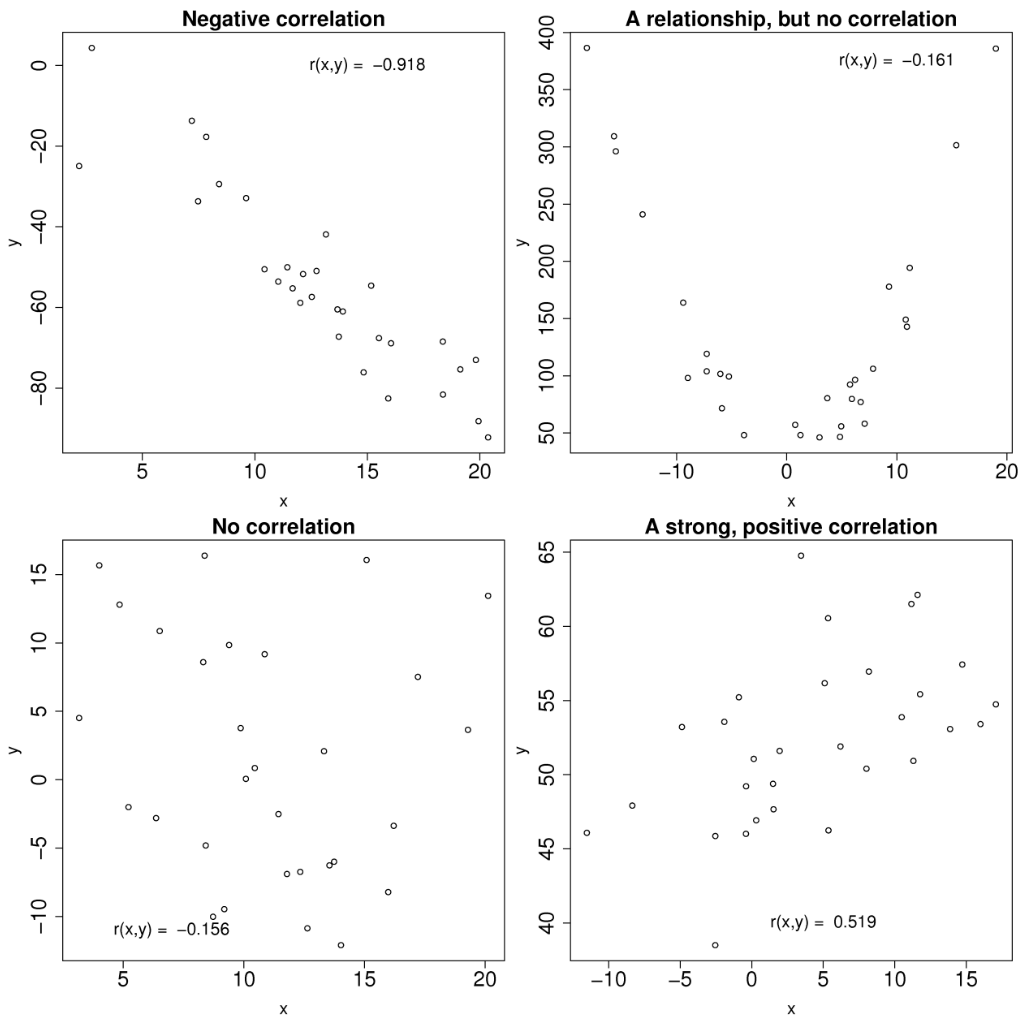
Review: correlation (cont.)

- Which one has highest/lowest/negative/positive correlation?
- Which one has (almost) no correlation?



- What does that mean if correlation of two variables is -1/+1?

Review: correlation (cont.)



Least squares? Least squares regression?

- *Regression* is the act of choosing the "best" values for the unknown parameters in a model on the basis of a set of measured data.
- Linear regression is the special case where the model is linear in the parameters. A straight line has the form:

$$y = a_0 + a_1 x + e$$

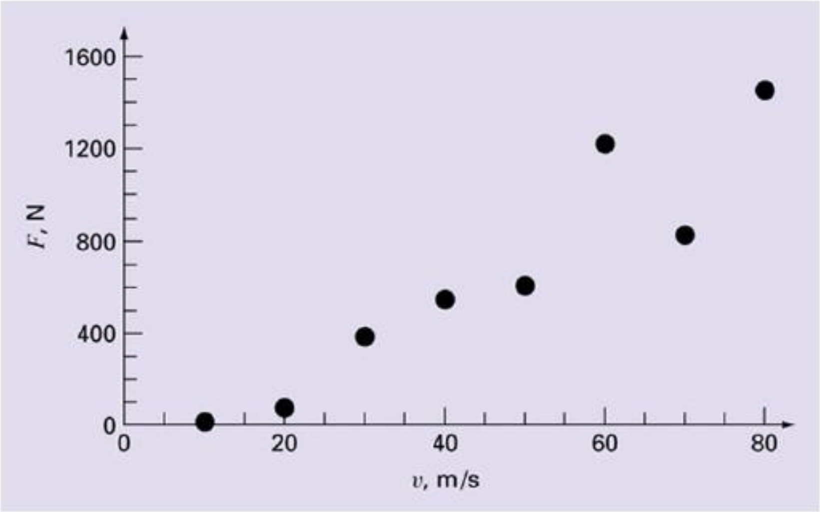
- There are many possible ways to define the "best" fit. However, the most commonly used measure for bestness is the sum of squared residuals.
  - Least sum of squares of errors → least squares in short.

Least squares (regression)

- It is the basis for :
  - DOE (Design of Experiments)
  - Latent variable methods
- We consider only 2 (sets of) variables : x and y (or x's and y)
  - Simple least squares
  - Multiple least squares
  - Generalized least squares

Simple least squares

- Wind tunnel example
  - How can we find the best line that describe the following data?



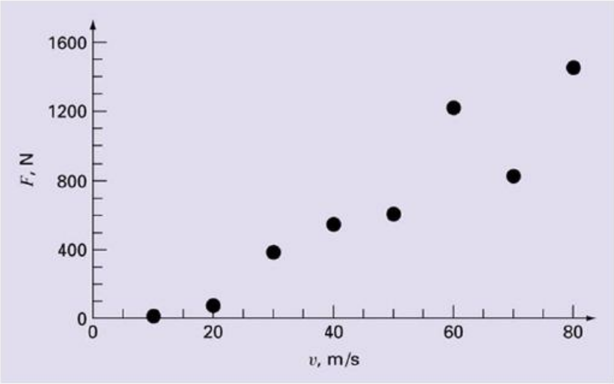
Data from wind tunnel experiments:
Drag force (F) at various wind velocities

v (m/s)	10	20	30	40	50	60	70	80
F (N)	25	70	380	550	610	1220	830	1450

Wind tunnel example (cont.)

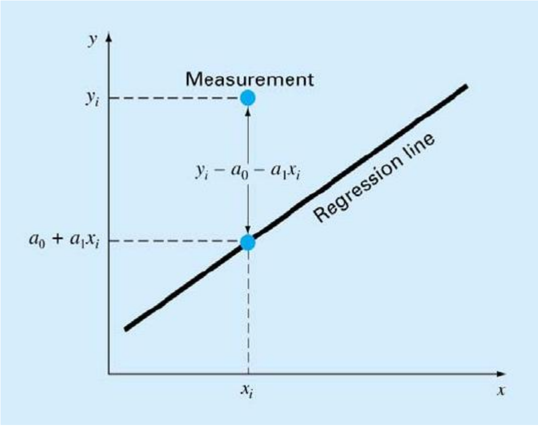
- From the plot, a linear line seems adequate.

  $y = a_0 + a_1 x + e$



- At a data point (x_i, y_i), error between the line and the point is: (see the figure on the right)

  $e_i = y_i - a_0 - a_1 x_i$



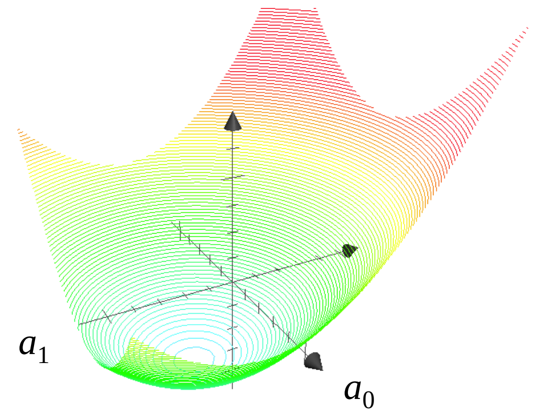
- Earlier, least squares means least sum of squares of errors. For all data points, sum of squares of errors is:

  $$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$$

- We need to find model parameters a_0 and a_1 that minimize S_r.
  - "Least squares"

Wind tunnel example (cont.)

- How to find model parameters?
  - Take a look at Sr. $S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$
  - S_r is a parabolic function w.r.t a_0 and a_1 and sign of a_o^2 and a_1^2 are plus.
  - S_r becomes minimum where



$$\frac{\partial S_r}{\partial a_0} = 0 \ \& \ \frac{\partial S_r}{\partial a_1} = 0.$$

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_i) \qquad \frac{\partial S_r}{\partial a_1} = -2\sum [(y_i - a_0 - a_1 x_i) x_i]$$

$$0 = \sum y_i - \sum a_0 - \sum a_1 x_i \qquad 0 = \sum x_i y_i - \sum a_0 x_i - \sum a_1 x_i^2$$

  - Rearranging and solving for a_0 and a_1

$$n a_0 + \left(\sum x_i\right) a_1 = \sum y_i \qquad \left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 = \sum x_i y_i$$

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \left(\sum x_i\right)^2} \qquad a_0 = \bar{y} - a_1 \bar{x}$$

Wind tunnel example (cont.)

- Calculations

v (m/s)	10	20	30	40	50	60	70	80
F (N)	25	70	380	550	610	1220	830	1450

i	x_i	y_i	x_i^2	$x_i y_i$
1	10	25	100	250
2	20	70	400	1,400
3	30	380	900	11,400
4	40	550	1,600	22,000
5	50	610	2,500	30,500
6	60	1,220	3,600	73,200
7	70	830	4,900	58,100
8	80	1,450	6,400	116,000
Σ	360	5,135	20,400	312,850

Wind tunnel example (cont.)

- Calculations

$$\bar{x} = \frac{360}{8} = 45 \qquad \bar{y} = \frac{5{,}135}{8} = 641.875$$

$$a_1 = \frac{8(312{,}850) - 360(5{,}135)}{8(20{,}400) - (360)^2} = 19.47024$$

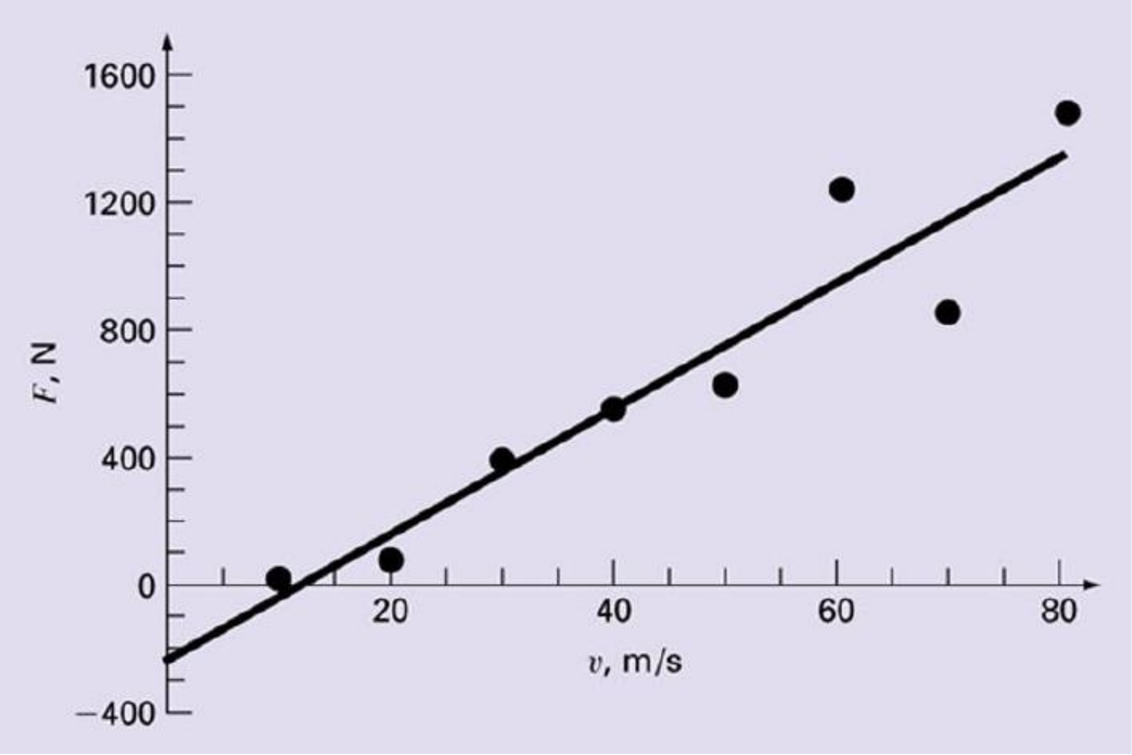
$$a_0 = 641.875 - 19.47024(45) = -234.2857$$

$$F = -234.2857 + 19.47024\,v$$

- This is called simple least squares.

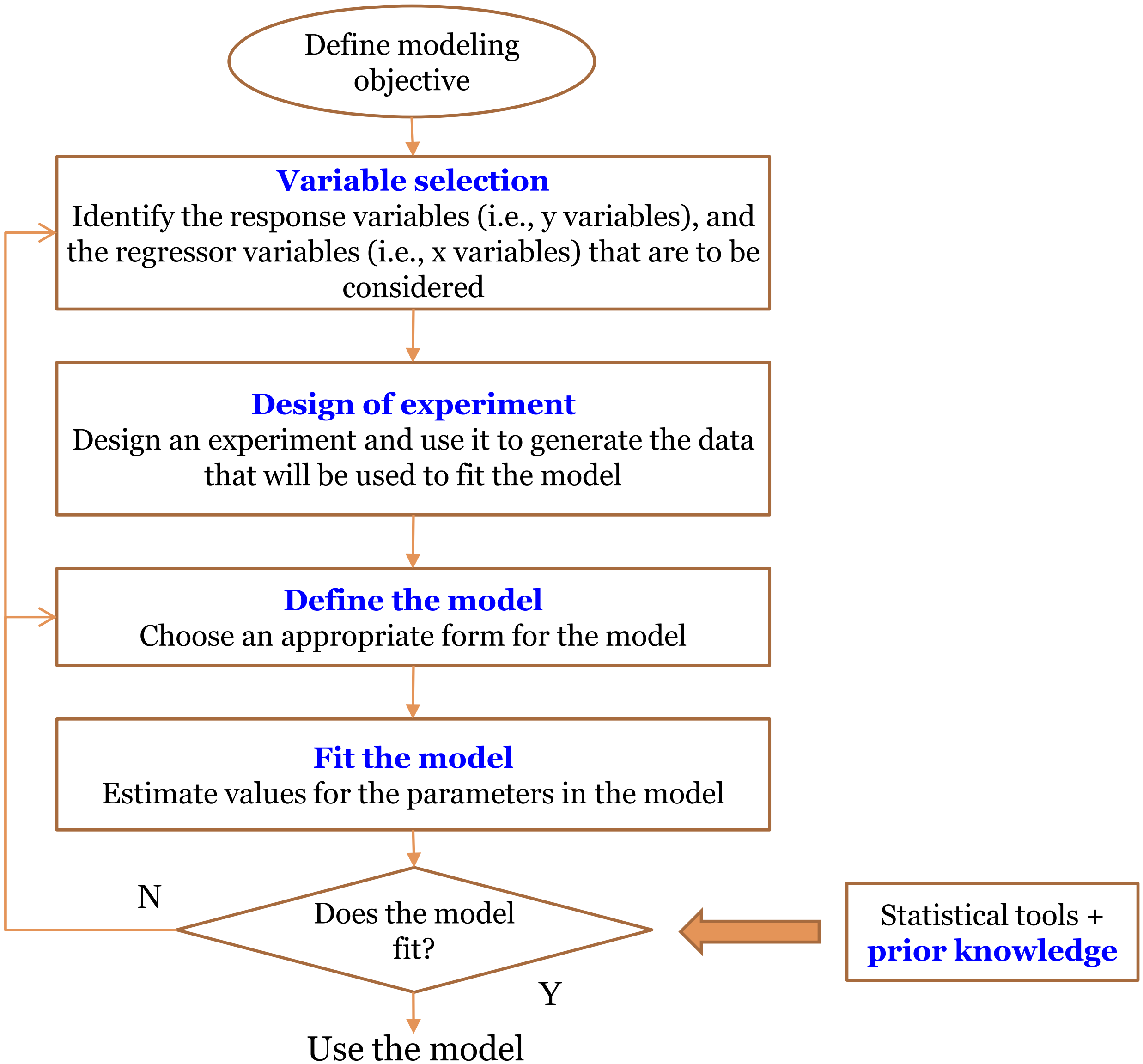
Wind tunnel example (cont.)

- Results



Is this OK with you?

General modeling procedure



Simple least squares

- Summary
  - Model form: $y = a_0 + a_1 x + e$
  - $S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2$ becomes minimizes where $\frac{\partial S_r}{\partial a_0} = 0 \; \& \; \frac{\partial S_r}{\partial a_1} = 0.$
  - Rearranging and solving for a_0 and a_1

$$n a_0 + \left(\sum x_i\right) a_1 = \sum y_i \qquad \left(\sum x_i\right) a_0 + \left(\sum x_i^2\right) a_1 = \sum x_i y_i$$

$$\Rightarrow \quad a_1 = \frac{n \sum x_i y_i - \sum x_i \sum y_i}{n \sum x_i^2 - \left(\sum x_i\right)^2} \qquad a_0 = \bar{y} - a_1 \bar{x}$$

- Question: what if our model we want to find is non-linear?

  Ex. Activation energy in rate constant

$$k = k_0 e^{-E/RT}$$

→ Linearize !

Linearization

- Want to model non-linear relationships between independent (x) and dependent (y) variables.
  1. Make a simple linear model through a suitable transformation.

$$y = f(x) + e \quad \rightarrow \quad y = a_0 + a_1 x + e$$

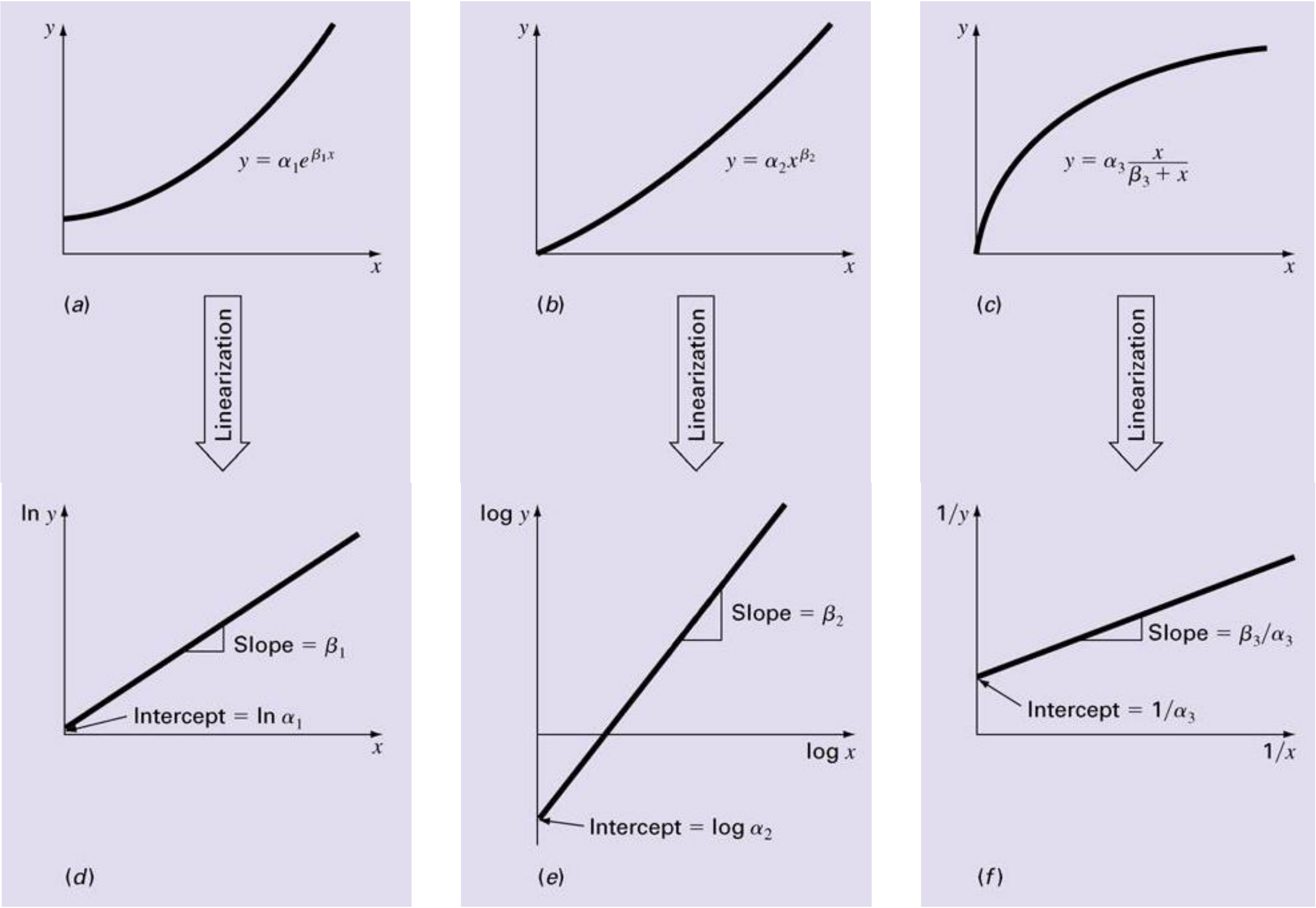
  2. Use previous results (simple least squares)

$$a_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x_i^2 - \left(\sum x_i\right)^2} \qquad a_0 = \bar{y} - a_1 \bar{x}$$

※Caution: transformation also changes P.D.F of variables (and errors)

We will discuss about this in model assessment.

Linearization (Cont.)



Polynomial regression

- For quadratic form

$$y = a_0 + a_1 x + a_2 x^2 + e$$

  - Sum of squares

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} \left(y_i - a_0 - a_1 x_i - a_2 x_i^2\right)^2$$

Again, S_r has a parabolic shape w.r.t a_0, a_1, and a_2. with plus signs of a_0^2, a_1^2, and a_2^2.

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum x_i (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum x_i^2 (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0$$

Polynomial regression (Cont.)

- Rearranging the previous equations gives

$$(n)a_0 + \left(\sum x_i\right)a_1 + \left(\sum x_i^2\right)a_2 = \sum y_i$$
$$\left(\sum x_i\right)a_0 + \left(\sum x_i^2\right)a_1 + \left(\sum x_i^3\right)a_2 = \sum x_i y_i$$
$$\left(\sum x_i^2\right)a_0 + \left(\sum x_i^3\right)a_1 + \left(\sum x_i^4\right)a_2 = \sum x_i^2 y_i$$

$$\Rightarrow \begin{pmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{pmatrix}$$

  the above equations can be solved easily. (three unknowns and three equations.)

- For general polynomials

$$y = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m + e$$

- From the results of two cases ($y = a_0 + a_1 x$ & $y = a_0 + a_1 x + a_2 x^2$)

$$\frac{\partial S_r}{\partial a_0} = \frac{\partial S_r}{\partial a_1} = \cdots = \frac{\partial S_r}{\partial a_m} = 0$$

  we need to solve (m+1) linear algebraic equations for (m+1) parameters.

Multiple least squares

- Consider when there are more than two independent variables, x_1, x_2, …, x_m. ➔ regression plane.

$$y = a_0 + a_1 x_1 + a_2 x_2 + \cdots + a_m x_m + e$$

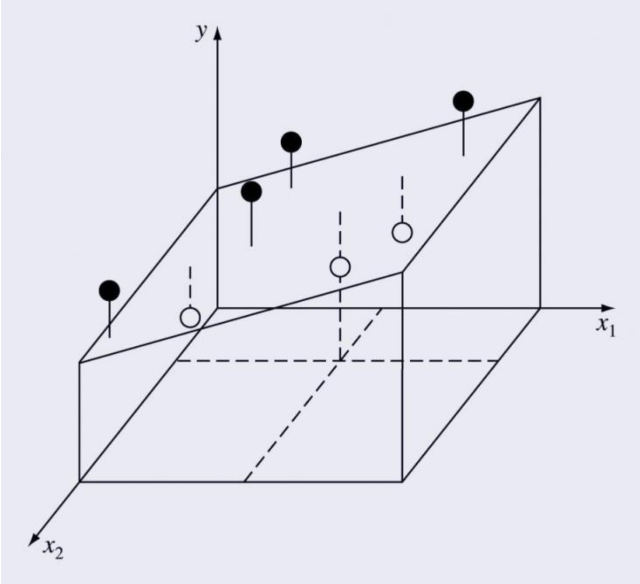
- For 2-D case, $y = a_0 + a_1 x_1 + a_2 x_2$.
  - Again, S_r has a parabolic shape w.r.t a_0, a_1, a_2

$$S_r = \sum (y_i - a_0 - a_1 x_{1,i} - a_2 x_{2,i})^2$$

$$\frac{\partial S_r}{\partial a_0} = -2\sum (y_i - a_0 - a_1 x_{1,i} - a_2 x_{2,i}) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2\sum x_{1,i}(y_i - a_0 - a_1 x_{1,i} - a_2 x_{2,i}) = 0$$

$$\frac{\partial S_r}{\partial a_2} = -2\sum x_{2,i}(y_i - a_0 - a_1 x_{1,i} - a_2 x_{2,i}) = 0$$



Multiple least squares (Cont.)

- Rearranging and solve for a_0, a_1 and a_2 gives

$$\begin{pmatrix} n & \sum x_{1,i} & \sum x_{2,i} \\ \sum x_{1,i} & \sum x_{1,i}^2 & \sum x_{1,i}x_{2,i} \\ \sum x_{2,i} & \sum x_{1,i}x_{2,i} & \sum x_{2,i}^2 \end{pmatrix} \begin{Bmatrix} a_1 \\ a_2 \\ a_3 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_{1,i}y_i \\ \sum x_{2,i}y_i \end{Bmatrix}$$

- For an m-dimensional plane,

$$y = a_0 + a_1 x_1 + a_2 x_2 + \cdots + a_m x_m + e$$

- Same as in general polynomials,

$$\frac{\partial S_r}{\partial a_0} = \frac{\partial S_r}{\partial a_1} = \cdots = \frac{\partial S_r}{\partial a_m} = 0$$

we need to solve $(m+1)$ linear algebraic equations for $(m+1)$ parameters.

General least squares

- The following form includes all cases (simple least squares, polynomial regression, multiple regression)

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

$$\text{where } z_0, z_1, \ldots, z_m \quad : m+1 \text{ different functions}$$

Ex. Simple and multiple least squares

$$Z_0 = 1, Z_1 = x_1, Z_2 = x_2, \cdots, Z_m = x_m$$

polynomial regression

$$Z_0 = x^0 = 1, Z_1 = x^1, Z_2 = x^2, \cdots, Z_m = x^m$$

- Same as before,

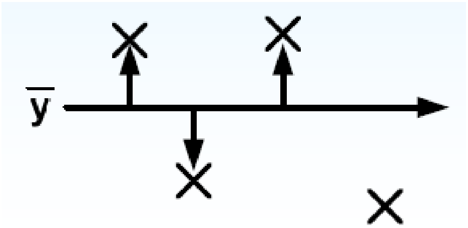
$$\frac{\partial S_r}{\partial a_0} = \frac{\partial S_r}{\partial a_1} = \cdots = \frac{\partial S_r}{\partial a_m} = 0$$

we need to solve (m+1) linear algebraic equations for (m+1) parameters.

Quantification of errors

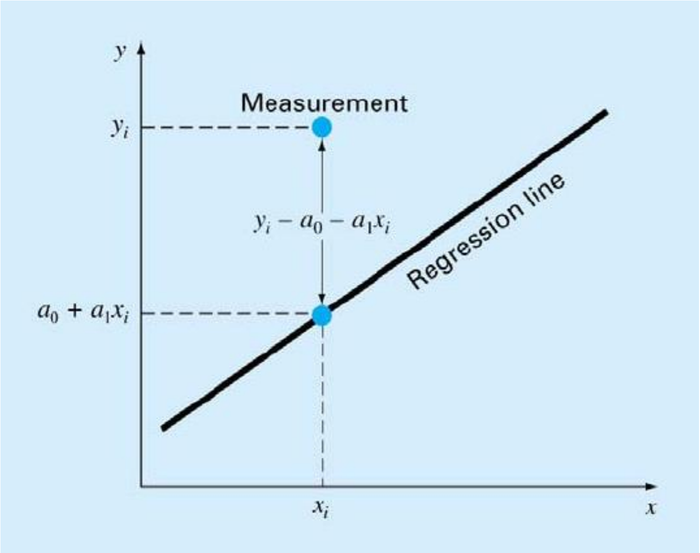
$$S_t = \sum (y_i - \bar{y})^2$$

Total sum of squares around the mean for the response variable, y



$$S_r = \sum e_i^2 = \sum \left(y_i - a_0 z_{0,i} - a_1 z_{1,i} - \cdots - a_m z_{m,i}\right)^2$$

Sum of squares of residuals around the regression line



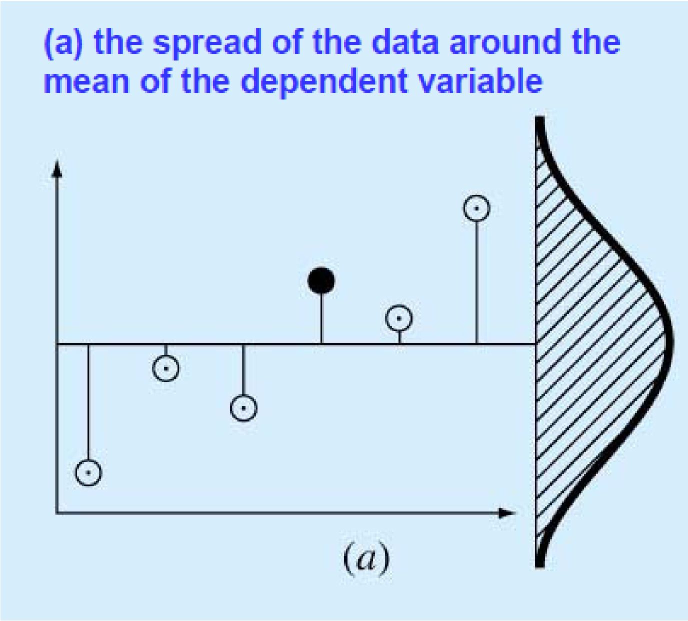
Quantification of errors (Cont.)

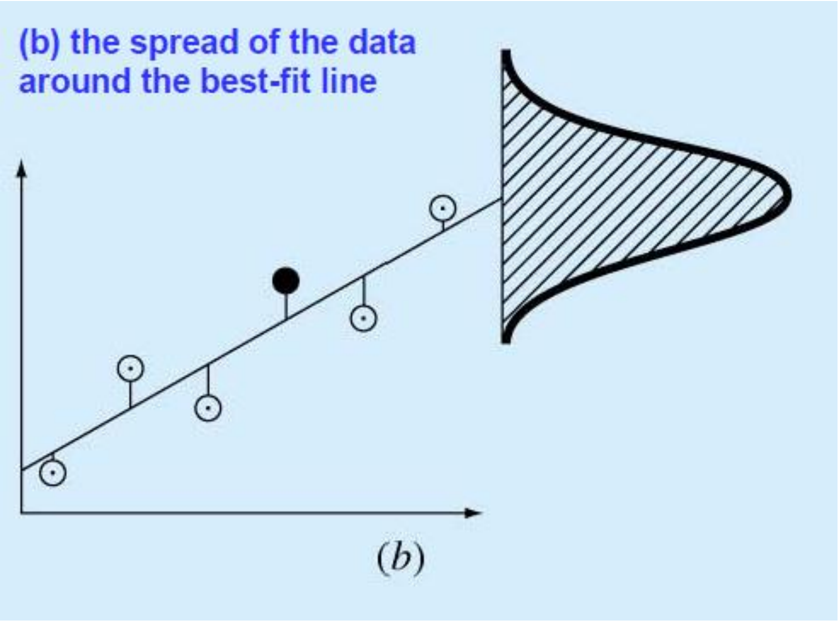
$$S_y = \sqrt{\frac{1}{n-1}\sum (y_i - \bar{y})^2} = \sqrt{\frac{S_t}{n-1}}$$

Standard deviation of *y*

$$S_{y/x} = \sqrt{\frac{S_r}{n-(m+1)}}$$

Standard error of predicted *y*
→ quantify appropriateness of regression





Quantification of errors (Cont.)

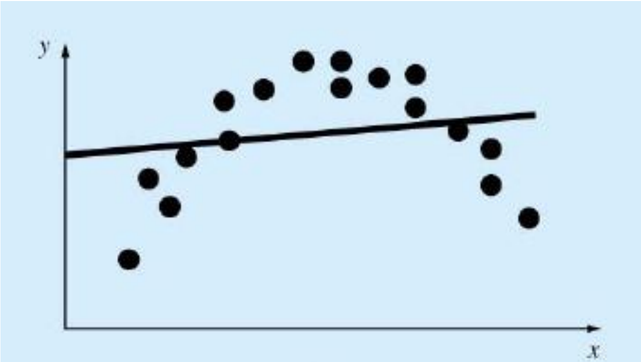
- Coefficients of determination, R^2

$$R^2 = \sqrt{\frac{S_t - S_r}{S_t}}$$

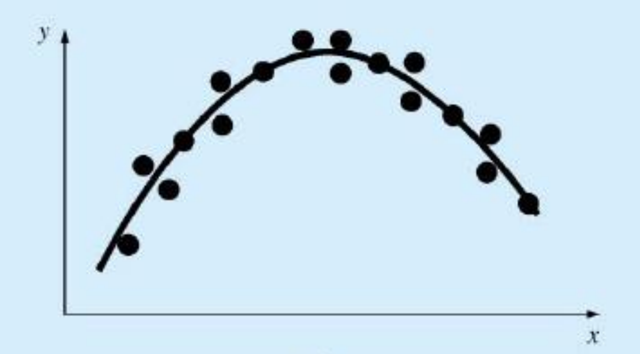
The amount of variability in the data explained by the regression model.

$R^2 = 1$ when $S_r = 0$: perfect fit (a regression curve passes through data points)

$R^2 = 0$ when $S_r = S_t$: as bad as doing nothing



(a)



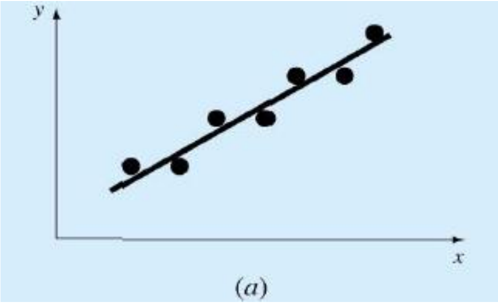
(b)

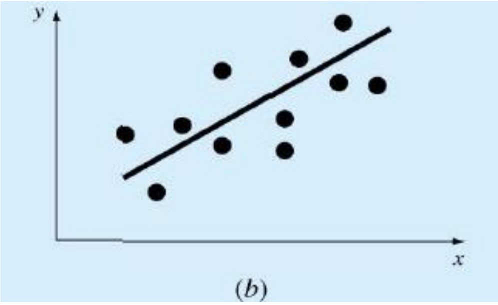
It is evident from the figures that a parabola is adequate.
R^2 of (b) is higher than that of (a)

Quantification of errors (Cont.)

- **Warning!** : $R^2 \approx 1$ **does not guarantee** that the model is adequate, nor the model will predict new data well.
  - It is possible to force R^2 to be one by adding as many terms as there are observations.
  - S_r can be big when variance of random error is large.

  (Usual assumption on error is that error is random is unpredictable)





Practice using Minitab

(1) Wind tunnel example with higher polynomials

(2) Simple regression with increasing random noise

Confidence intervals - coefficients

- Coefficients in the regression model have confidence interval.

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

  - Why? They are also statistics like $\bar{x}$ & s. That is, they are numerical quantities calculated in a sample (not entire population). They are estimated values of parameters.

Statistic that we want to find its confidence interval

$$statistic \pm A \times \sigma_{statistic}$$

Value that depends on P.D.F of the statistic & confidence level α

Standard error of the statistic

statistic	A	$\sigma_{statistic}$
$\bar{x}$	$z_{\alpha/2}$	$\sigma_x / \sqrt{n}$
$\bar{x}$	$t_{\nu,\alpha/2}$	$s_x / \sqrt{n}$

※The standard error of a statistic is the standard deviation of the sampling distribution of that statistic

Confidence intervals – coefficients (cont.)

- Matrix representation of GLS

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

$$\Rightarrow \quad \mathbf{y} = \mathbf{Z}\mathbf{a} + \mathbf{e}$$

– matrix of the calculated values of the basis functions at the measured values of the independent variable

– observed valued of the dependent variable

– unknown coefficients

– residuals

$$\mathbf{Z} = \begin{bmatrix} Z_{01} & Z_{11} & \cdots & Z_{m1} \\ Z_{02} & Z_{12} & \cdots & Z_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ Z_{0n} & Z_{1n} & \cdots & Z_{mn} \end{bmatrix} \quad \begin{aligned} \mathbf{y}^T &= \lfloor y_1 \ \ y_2 \ \ \cdots \ \ y_n \rfloor \\ \mathbf{a}^T &= \lfloor a_0 \ \ a_1 \ \ \cdots \ \ a_m \rfloor \\ \mathbf{e}^T &= \lfloor e_1 \ \ e_2 \ \ \cdots \ \ e_n \rfloor \end{aligned}$$

m+1: number of coefficients
n: number of data points

Confidence intervals – coefficients (Cont.)

- Example

Fitting quadratic polynomials to five data points

x	-1.0	-0.5	0.0	0.5	1.0
y	1.0	0.5	0.0	0.5	2.0

$$y = a_0 + a_1 x + a_2 x^2 + e$$

$$\mathbf{y} = \mathbf{Za} + \mathbf{e}$$

$$\begin{bmatrix} 1.0 \\ 0.5 \\ 0.0 \\ 0.5 \\ 2.0 \end{bmatrix} = \begin{bmatrix} 1 & -1.0 & 1.0 \\ 1 & -0.5 & 0.25 \\ 1 & 0.0 & 0.0 \\ 1 & 0.5 & 0.25 \\ 1 & 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \\ e_5 \end{bmatrix}$$

Three unknowns
Five equations

Can you solve this problem?

Confidence intervals – coefficients (Cont.)

- Solutions

$\mathbf{y} = \mathbf{Z}\mathbf{a} + \mathbf{e}$

Sum of squares of errors

$$S_r = \sum e_i^2 = \mathbf{e}^T\mathbf{e} = (\mathbf{y} - \mathbf{Z}\mathbf{a})^T(\mathbf{y} - \mathbf{Z}\mathbf{a})$$

$$\frac{\partial S_r}{\partial \mathbf{a}} = 0 \longrightarrow (\mathbf{Z}^T\mathbf{Z})\mathbf{a} = \mathbf{Z}^T\mathbf{y}$$

Called "normal equations"

1. LU decomposition or other methods to solve L.A.E

$$(\mathbf{Z}^T\mathbf{Z})\mathbf{a} = \mathbf{Z}^T\mathbf{y} \qquad \Rightarrow \text{"}\mathbf{A}\mathbf{x} = \mathbf{b}\text{"}$$

2. Matrix inversion

$$(\mathbf{Z}^T\mathbf{Z})\mathbf{a} = \mathbf{Z}^T\mathbf{y} \qquad \Rightarrow \mathbf{a} = (\mathbf{Z}^T\mathbf{Z})^{-1}\mathbf{Z}^T\mathbf{y}$$

computationally not efficient, but statistically useful

Confidence intervals – coefficients (Cont.)

- Matrix inversion approach

$$\mathbf{a} = \left(\mathbf{Z}^T\mathbf{Z}\right)^{-1}\mathbf{Z}^T\mathbf{y}$$

Denote Z_{ii}^{-1} as the diagonal element of $\left(\mathbf{Z}^T\mathbf{Z}\right)^{-1}$

Confidence interval of estimated coefficients

$$a_{i-1} \pm t_{n-(m+1),\alpha/2}\sqrt{S_{y/x}^2 Z_{ii}^{-1}}$$

$t_{n-(m+1),\alpha/2}$ Student t statistics

$S_{y/x} = \sqrt{\dfrac{S_r}{n-(m+1)}}$ Standard error of estimate

Minitab exercise with the wind tunnel example

What if confidence intervals contain zero?

Model assessment

- When we do not know the model form, we have to assess the model before use it after we fit a regression model.
  - However, in order to assess the model and make inferences about the parameters and predictions from the model, we will have to employ statistics and make some assumptions about the nature of the disturbance.
- Tools for model assessment
  - $S_{y/x}$, R^2 (quantitative) (→ not recommended)
  - Residual Plots (qualitative)
  - Normal probability chart (qualitative or quantitative)
  - Test for lack of fit (quantitative)
    - This is used when the dataset includes replicates. It is based on analysis of variance (ANOVA).

Model assessment - assumptions

- What is the most desirable errors in regression ?

$$y = a_0 z_0 + a_1 z_1 + a_2 z_2 + \cdots + a_m z_m + e$$

- Assumptions on error
  - Error is additive $y = a_0 + a_1 x_1 + e$ ~~$y = (a_0 + a_1 x_1)e$~~
  - The variance of the error is constant and is not related to values of the response or values of the regressor variables.
  - There is no error associated with the values of the regressor variables.
  - Error is a random variable with Gaussian distribution $N(0,\sigma^2)$ (σ^2 usually unknown)

Model assessment – residual plots

- Recall the assumptions on error
  - Error is not related to the values of response or regressor variables.

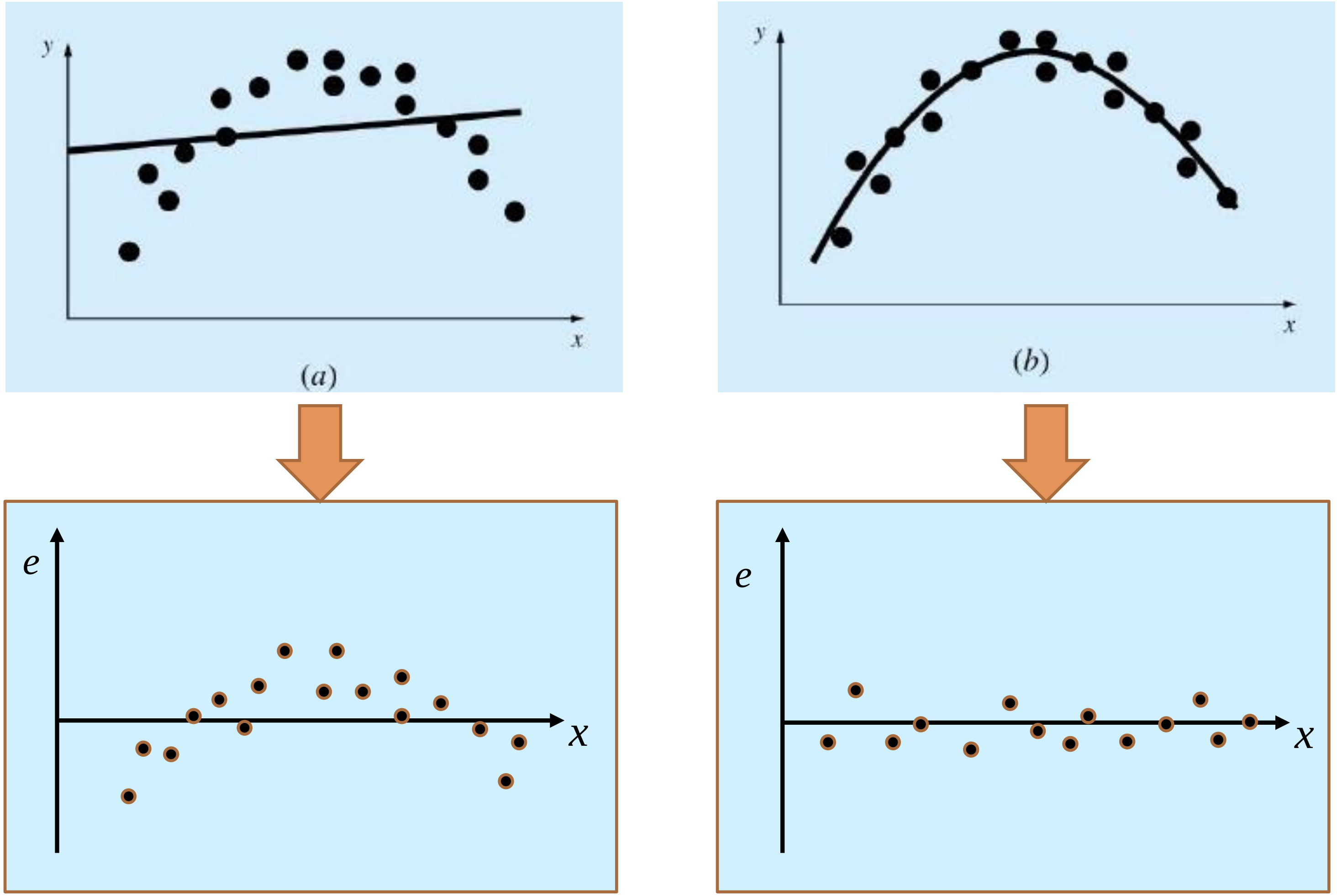
Then, assumptions will not be valid if the model is wrong.

- Following residual plots will reveal this.
  - Residuals vs. regressor variables
  - Residuals vs. fitted y values
  - Residuals vs. "lurking" variables (i.e. time or order)

  → These plots will show "some patterns" when a model is inadequate.

Model assessment – residual plots

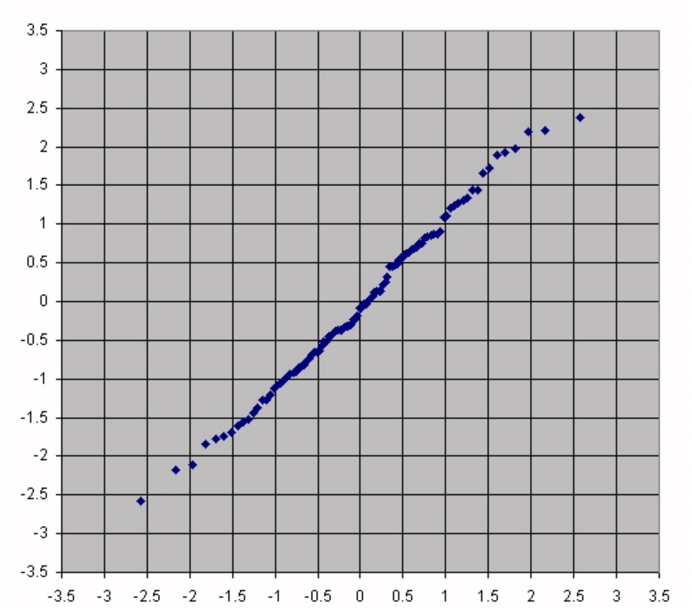
- Examples



Model assessment – normal probability plot

- Recall the assumptions on error
  - Error is a random variable with Gaussian distribution $N(0, \sigma^2)$ (σ^2 usually unknown)

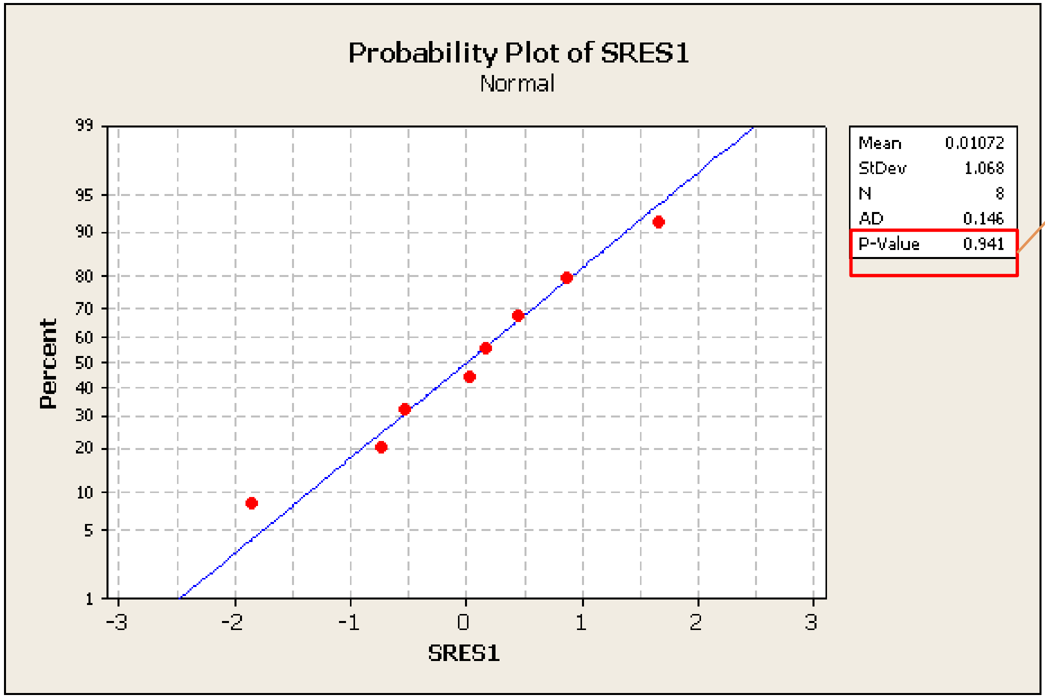
Then, errors will fall onto a straight line (y = x) in a normal probability plot. (especially useful when the number of data points is large)



Normal probability plot

Model assessment – normal probability plot

- Using normality test. (hypothesis test)
  - Quantitative. Useful when data are small.
    - H_o : data is normally distributes.
    - H_1 : data is NOT normally distributed.

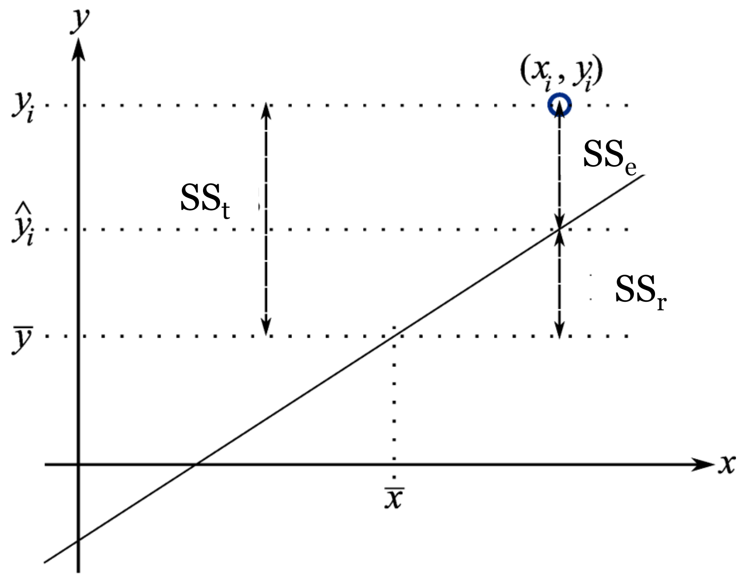


At α levels greater than 0.941, there is evidence that the data do not follow a normal distribution.

Model assessment – ANOVA (Test for lack of fit)

- The variance breakdown

$$SS_t = \sum (y_i - \bar{y})^2$$



$$SS_e = \sum (y_i - \hat{y}_i)^2$$

$$SS_r = \sum (\hat{y}_i - \bar{y})^2$$

- Ratio of SS_r/SS_e follows F distribution when corrected with degree of freedom.
- If regression is **not** meaningful, the ratio (SS_r/SS_e) is small and $SS_t \fallingdotseq SS_e$.

Model assessment – ANOVA (Test for lack of fit)

ANOVA Table

Source of Var.	Sum of Squares	Degrees of Freedom	Mean Square	F_0
Regression	SS_R	p	$MS_R=SS_R/p$	MS_R/ MS_E
(Residual) error	SS_E	n-p	$MS_E=SS_E/(n-p)$	
Total	SS_t	n-1		

Compare F_0 to the critical value $F_{p,n-p;\alpha}$

What we are doing is a *test of hypothesis*.
We are testing the hypothesis:

$$H_0 : \beta_0 = \cdots = \beta_p = 0$$

H_1 : at least one parameter is not equal to zero.

[FYI]Meaning of a p-value in hypothesis test

- A measure of how much evidence we have against the null hypothesis.
  - Null hypothesis (H_0) represents the hypothesis of no change or no effect.
  - Much research involves making a hypothesis and then collecting data to test that hypothesis. Then researchers will collect data and measure the consistency of this data with the null hypothesis.
  - A small p-value is evidence against the null hypothesis while a large p-value means little or no evidence against the null hypothesis.
  - Traditionally, researchers will reject a null hypothesis if the p-value is less than 0.05 ($\alpha = 0.05$).

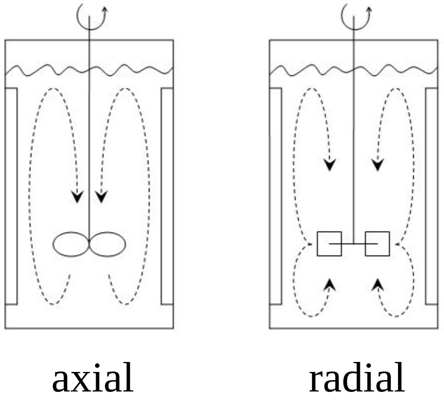
  → p-value can mean that the possibility that you can be wrong when rejecting the null hypothesis.

Integer variables in the model

- Integer variables 0 and 1 can represent qualitative variables.
  - Example: raw material from Spain, India, or Vietnam
    - $y = a_0 + a_1x_1 + \ldots + a_kx_k + r_1d_1 + r_2d_2 + r_3d_3$
    - $d_1 = 1$ and $d_2 = 0$ and $d_3 = 0$ for Spain
    - $d_1 = 0$ and $d_2 = 1$ and $d_3 = 0$ for India
    - $d_1 = 0$ and $d_2 = 0$ and $d_3 = 1$ for Vietnam
- Often called indicator variables for this reason

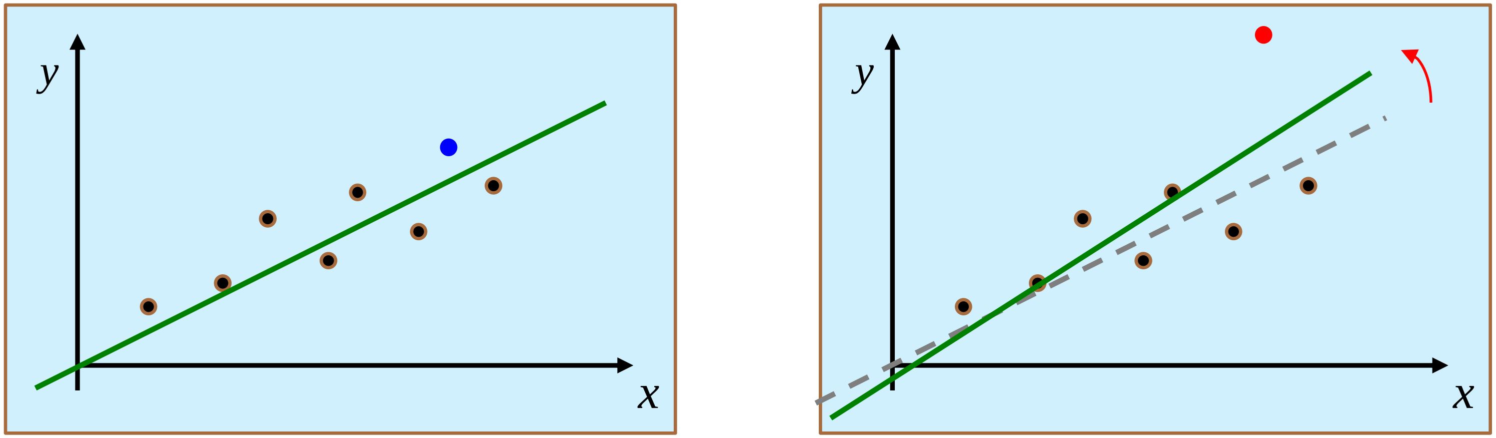
Integer variables in the model

- Example
  - Want to predict yield when two different impeller used. Yield = *f*(temperature, impeller type)
  - Build two different models (one for axial, one for radial)
  - Build one model using indicator variable. $y = a_0 + a_1T + rd$
    - $y = a_0 + a_1T + rd_i$
    - $d_i = 0$ for axial, $d_i = 1$ for radial



Leverage effect

- Unusual observations influence the model parameters and our interpretation



Outliers have an over-proportional effect on resulting regression curves.

- To avoid the leverage effect,
  - Remove outliers before regression (but do not delete without investigation)
  - Use different S_r (no longer least squares)

Causal relation and correlation

- Causal relation
  - Cause and effect relation
    - Has physical/chemical/engineering meanings
  - x and y are **not** interchangeable
    - Direction exists.
- Correlation
  - (Linear) relationship between two variables
  - No physical/chemical/engineering meanings.
    - Average height of 20's men vs. year
  - x and y are interchangeable

Home work (1주일 후 강의시간에 제출할 것. 5 페이지 초과시 0점 처리)

표 1.2는 벤젠에 대한 온도에 따른 증기압 데이터이다. 몇몇 설계 계산에서 이 데이터를 대수 식으로 정확하게 상관시키는 것이 요구된다.

표 1.2: 벤젠의 증기압(Perry et al. [5]

온도, T (°C)	압력, P (mmHg)
-36.7	1
-19.6	5
-11.5	10
-2.6	20
+7.6	40
15.4	60
26.1	100
42.2	200
60.6	400
80.1	760

(a) 절대 온도를 독립변수로 하고 P를 종속변수로 가정하여 데이터를 서로 다른 차수로 상관지어라. 데이터를 가장 잘 맞추는 다항식 차수를 결정하라.

(b) Clapeyron 식을 사용하여 데이터를 상관지어라.

$$\log P_v = -\frac{\Delta H_v}{RT} + B$$

(c) Reidel 식을 사용하여 데이터를 상관지어라.

(이때 β는 2로 할 것.)

$$\log(P) = A + \frac{B}{T} + C\log(T) + DT^{\beta}$$

(d) 위의 상관식 중에서 어느 것이 주어진 데이터를 가장 잘 맞추는지에 대하여 논의하라.