Lecture # 37

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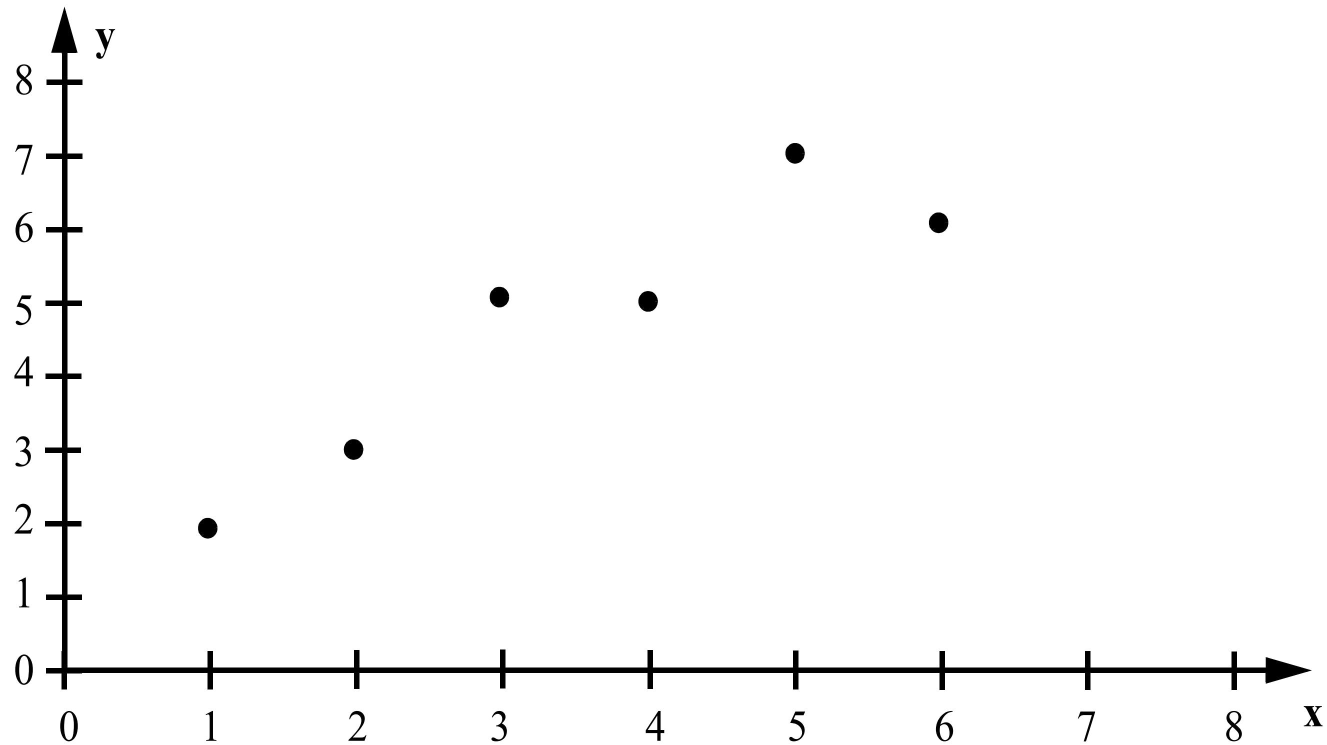
Nov. 28, 2005

Linear Regression



Modeling

To describe the data above, propose the model:

$$y = B_0 + B_1 x + \varepsilon$$

Fitted model will then be $\hat{y} = b_0 + b_1 x$

Want to select values for $b_0 \,\&\, b_1$ **that minimize**

$$\sum_{i=1}^{n=6} (y_i - \hat{y}_i)^2$$

Modeling (Cont.)

Define $$S(b_0, b_1) = \sum_{i=1}^{n=6} (y_i - \hat{y}_i)^2$$

the model residual Sum of Squares.

Minimize

$$S(b_0, b_1) = \sum_{i=1}^{n=6} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n=6} (y_i - b_0 - b_1 x_1)^2$$

Modeling (Cont.)

To find minimum S, take partial derivatives of S with respect to b_0 & b_1, set these equal to zero, and solve for b_0 & b_1

$$\frac{\partial}{\partial b_0} S(b_0, b_1) = 2\Sigma(y_i - b_0 - b_1 x_i)(-1) = 0$$

$$\frac{\partial}{\partial b_1} S(b_0, b_1) = 2\Sigma(y_i - b_0 - b_1 x_i)(-x_i) = 0$$

Modeling (Cont.)

$$-\Sigma y_i + \Sigma b_o + \Sigma b_1 x_i = 0$$

$$-\Sigma x_i y_i + \Sigma b_o x_i + \Sigma b_1 x_i^2 = 0$$

Simplifying, we obtain:

$$nb_0 + b_1 \Sigma x_i = \Sigma y_i$$

$$b_0 \Sigma x_i + b_1 \Sigma x_i^2 = \Sigma x_i y_i$$

Modeling (Cont.)

These two equations are known as "Normal Equations".

The values of $b_0 \;\&\; b_1$ that satisfy the Normal Equations are the least squares estimates -- they are the values that give a minimum S.

Matrix Form

$$\begin{bmatrix} N & \Sigma x_i \\ \Sigma x_i & \Sigma x_i^2 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \end{Bmatrix} = \begin{Bmatrix} \Sigma \; y_i \\ \Sigma \; x_i y_i \end{Bmatrix}$$

$$\begin{Bmatrix} b_0^* \\ b_1^* \end{Bmatrix}$$ **= Least Squares Estimates**

$$= \begin{bmatrix} n & \Sigma x \\ \Sigma x & \Sigma x^2 \end{bmatrix}^{-1} \begin{Bmatrix} \Sigma \; y \\ \Sigma \; xy \end{Bmatrix}$$

Matrix Form (Cont.)

$$\begin{Bmatrix} b_0^* \\ b_1^* \end{Bmatrix} = \frac{1}{n\Sigma x^2 - (\Sigma x)^2} \begin{bmatrix} \Sigma x^2 & -\Sigma x \\ -\Sigma x & n \end{bmatrix} \begin{Bmatrix} \Sigma \ y \\ \Sigma \ xy \end{Bmatrix}$$

$$= \frac{1}{n\Sigma x^2 - (\Sigma x)^2} \begin{bmatrix} \Sigma x^2 \Sigma y - \Sigma x \Sigma xy \\ -\Sigma x \Sigma y + n\Sigma xy \end{bmatrix}$$

Matrix Form (Cont.)

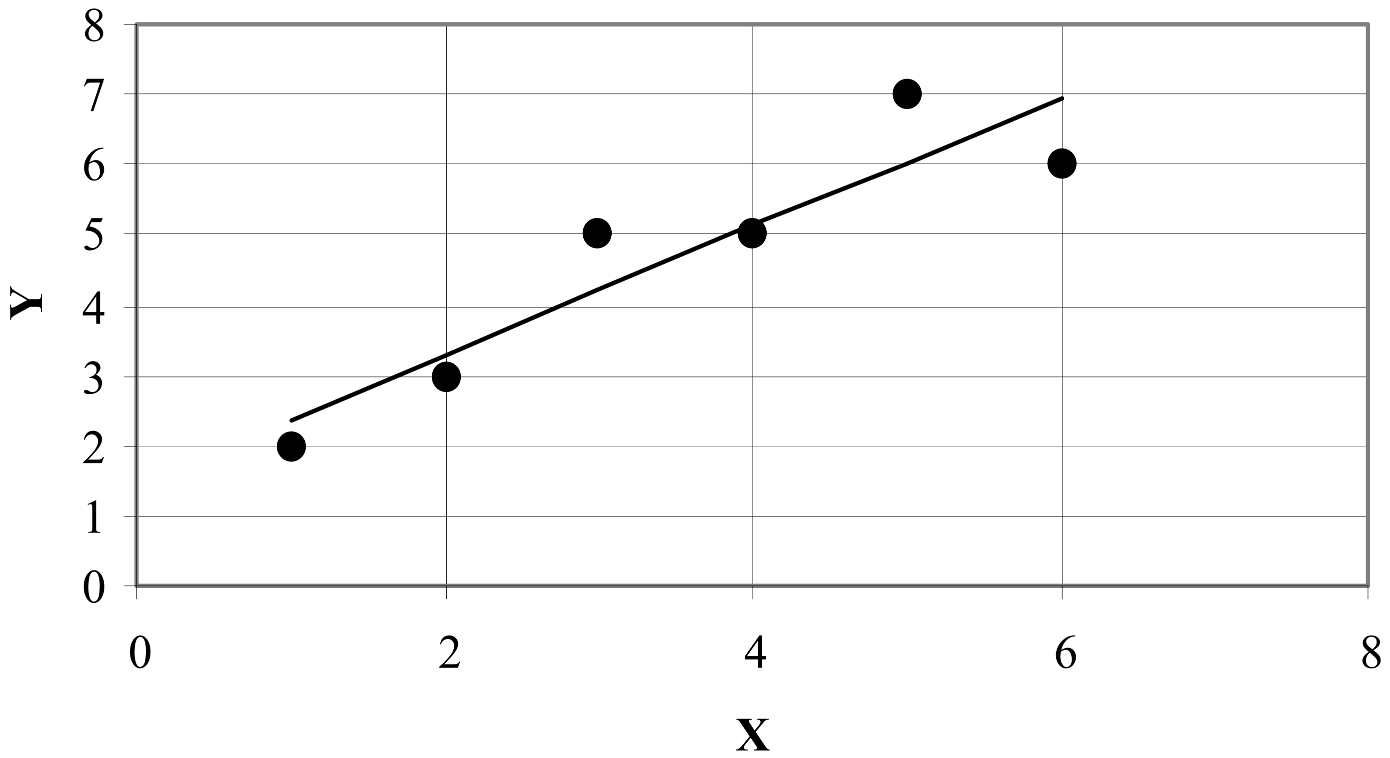
$$\begin{Bmatrix} b_0^* \\ b_1^* \end{Bmatrix} = \begin{bmatrix} 1.4667 \\ 0.9143 \end{bmatrix}$$

b_0^*, b_1^* are the values of b_0 & b_1 that minimize S, the Residual Sum of Squares.

$b_0^* = \hat{B}_0$ = an estimate of B_0

$b_1^* = \hat{B}_1$ = an estimate of B_1

Fitted Line



Matrix Approach

$\underset{\sim}{y}$: **Vector of Observations =** $\begin{bmatrix} 2 \\ 3 \\ 5 \\ 5 \\ 7 \\ 6 \end{bmatrix}$,

$\underset{\sim}{x}$: **Matrix of Independent Variables, i.e.,**

the Design Matrix = $\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \\ 1 & 5 \\ 1 & 6 \end{bmatrix}$

Matrix Approach (Cont)

$\underset{\sim}{\hat{y}}$ **= Vector of Predictions =** $\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \vdots \\ \hat{y}_n \end{bmatrix}$ **=** $\underset{\sim}{x}\underset{\sim}{b}$

b coefficients = $\begin{bmatrix} b_0 \\ b_1 \end{bmatrix}$

Matrix Approach (Cont.)

$\underset{\sim}{e}$ **= Vector of Prediction Errors =** $\begin{bmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{bmatrix}$

$\underset{\sim}{e}$ **=** $\underset{\sim}{y} - \underset{\sim}{\hat{y}}$

Want to Min $\underset{\sim}{e}^T \underset{\sim}{e}$ **or Min** $(\underset{\sim}{y} - \underset{\sim}{x}\underset{\sim}{b})^T(\underset{\sim}{y} - \underset{\sim}{x}\underset{\sim}{b})$

Matrix Approach (Cont.)

Take derivative with respect to b's and set = 0

$$-\underset{\sim}{x}^T(\underset{\sim}{y} - \underset{\sim}{x}\underset{\sim}{b}) = 0 = -\underset{\sim}{x}^T\underset{\sim}{y} + (\underset{\sim}{x}^T\underset{\sim}{x})\underset{\sim}{b}$$

$$(\underset{\sim}{x}^T\underset{\sim}{x})\underset{\sim}{b} = \underset{\sim}{x}^T\underset{\sim}{y}$$

Matrix Approach (Cont.)

Therefore, $\underset{\sim}{b} = (\underset{\sim}{x}^T \underset{\sim}{x})^{-1} \underset{\sim}{x}^T \underset{\sim}{y}$ **.**

It is analogous to $\begin{Bmatrix} b_0 \\ b_1 \end{Bmatrix} = \begin{bmatrix} n & \Sigma x \\ \Sigma x & \Sigma x^2 \end{bmatrix}^{-1} \begin{Bmatrix} \Sigma y \\ \Sigma xy \end{Bmatrix}$

Matrix Approach (Cont.)

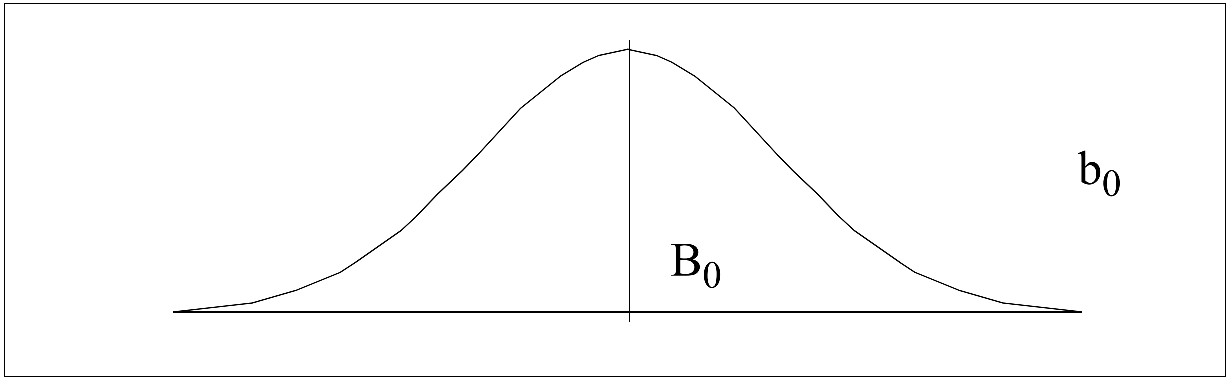
Re-run experiments several times

$$\begin{Bmatrix} b_0 \\ b_1 \end{Bmatrix} = \begin{Bmatrix} 1.4667 \\ 0.9143 \end{Bmatrix}, \begin{Bmatrix} b_0 \\ b_1 \end{Bmatrix} = \begin{Bmatrix} 1.5309 \\ 0.9741 \end{Bmatrix}, \begin{Bmatrix} b_0 \\ b_1 \end{Bmatrix} = \begin{Bmatrix} 1.5512 \\ 1.0134 \end{Bmatrix}$$

If true model is $y = B_0 + B_1 x + \varepsilon$

Then $E(b_0) = B_0$, $E(b_1) = B_1$, $E[\underset{\sim}{b}] = \underset{\sim}{B}$

Matrix Approach (Cont.)



$$Var(\underset{\sim}{b}) = (\underset{\sim}{x}^T \underset{\sim}{x})^{-1} \sigma_y^2$$

where, σ_y^2 describes the experimental error variation in the y's (σ_ε^2).

Matrix Approach (Cont.)

For our example, $Var(\underset{\sim}{b}) = \begin{bmatrix} \text{Var}(b_0) & \text{Cov}(b_0, b_1) \\ \text{Cov}(b_0, b_1) & \text{Var}(b_1) \end{bmatrix}$ **.**

If σ_y^2 **(or** σ_ε^2 **) is unknown, we can estimate it with**

$$s^2 = \frac{(y-\hat{y})^T (y-\hat{y})}{(\text{n - \# of parameters})} = \frac{e^T e}{n-p} = \frac{S_{res}}{\nu}$$

Matrix Approach (Cont.)

For the example,

$$s_y^2 = \frac{\sum_{i=1}^{n=6} (y_i - \hat{y}_i)^2}{n-2} = 0.67619$$

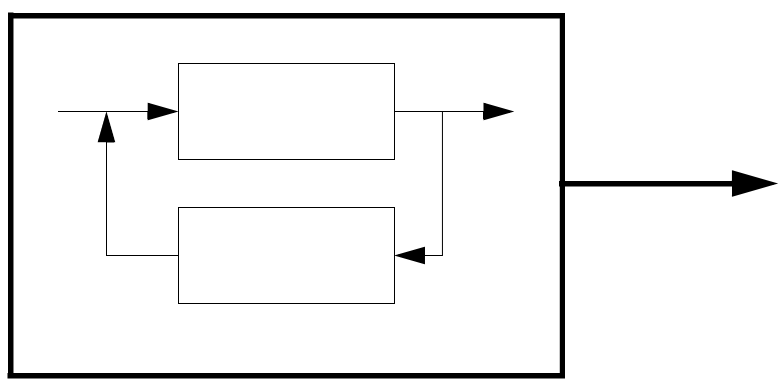
$$\widehat{\mathrm{Var}}(\underset{\sim}{b}) = (\underset{\sim}{x}^T \underset{\sim}{x})^{-1} s_y^2 = \begin{bmatrix} 0.586 & -0.135 \\ -0.135 & 0.039 \end{bmatrix}$$

$s_{b_0}^2 = 0.586, \quad s_{b_0} = 0.767$ **standard error of b_0**

$s_{b_1}^2 = 0.039, \quad s_{b_1} = 0.197$ **standard error of b_1**

Dynamic Systems

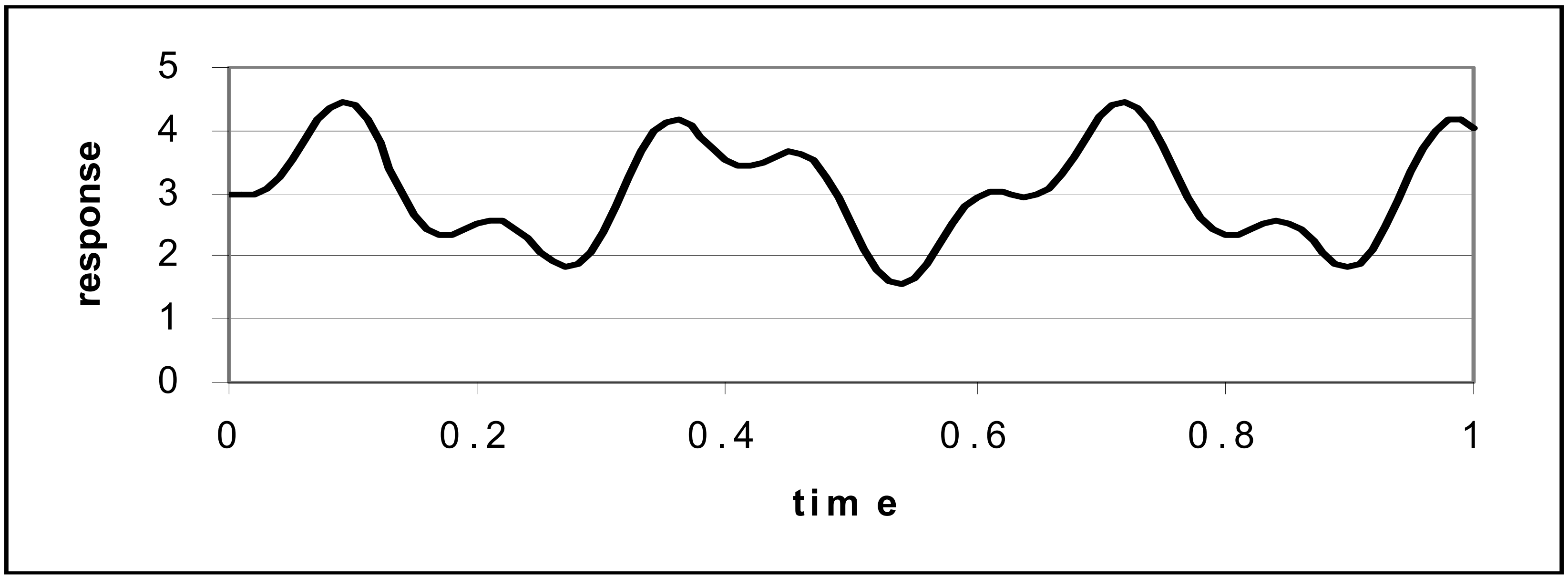
- Many processes have dynamic characteristics -- data are produced as a result of dynamic behavior within the process
  - Chemical processes
  - Vibrating systems
  - ?



Process Data, X's

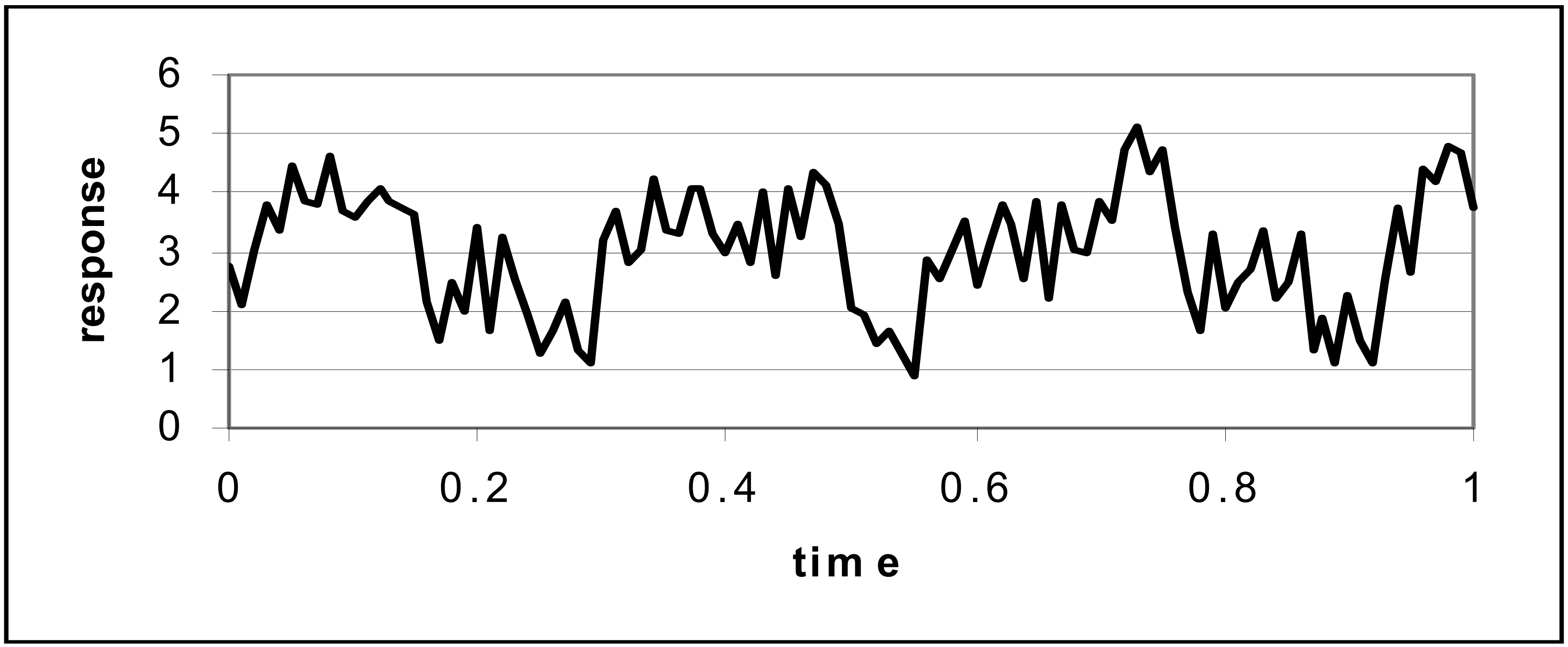
More on Dynamic Systems

- Because of our experience with differential equations and vibrations, we tend to think of dynamic behavior as in the figure below.



Common Cause Variability

- **With the addition of process noise, however, we often see behavior like that below.**

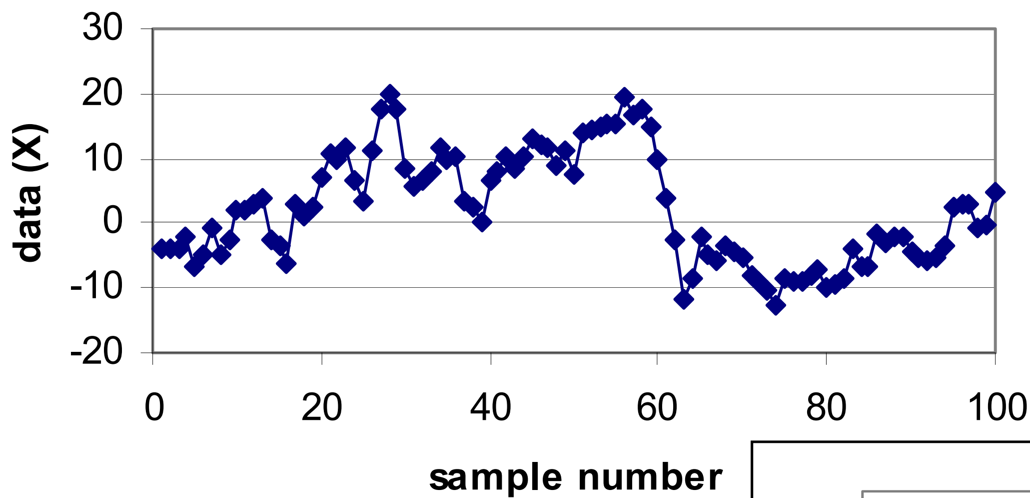


Time Series Analysis

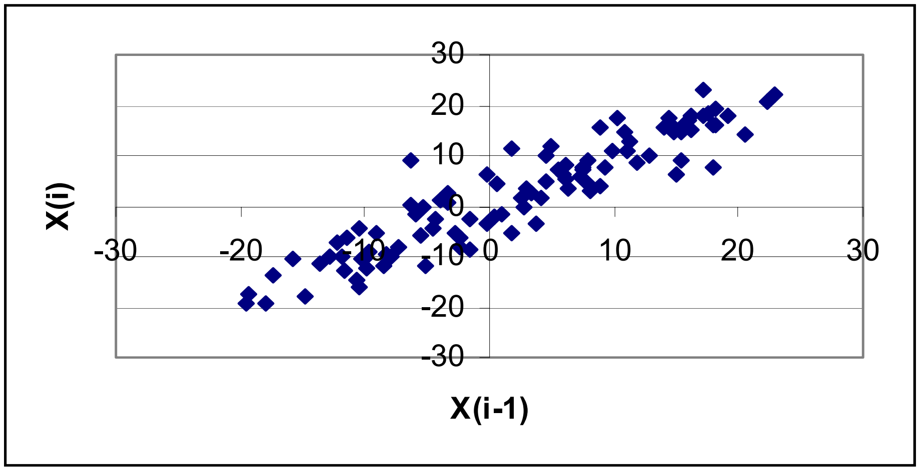
- For situations like that shown in the previous figure, we can use time series analysis to extract information about the process.
- From a time series model we can "back out" information about the unknown underlying system dynamics.
- Simple autoregressive model [AR(1)]

$$X_i = \phi X_{i-1} + a_i$$

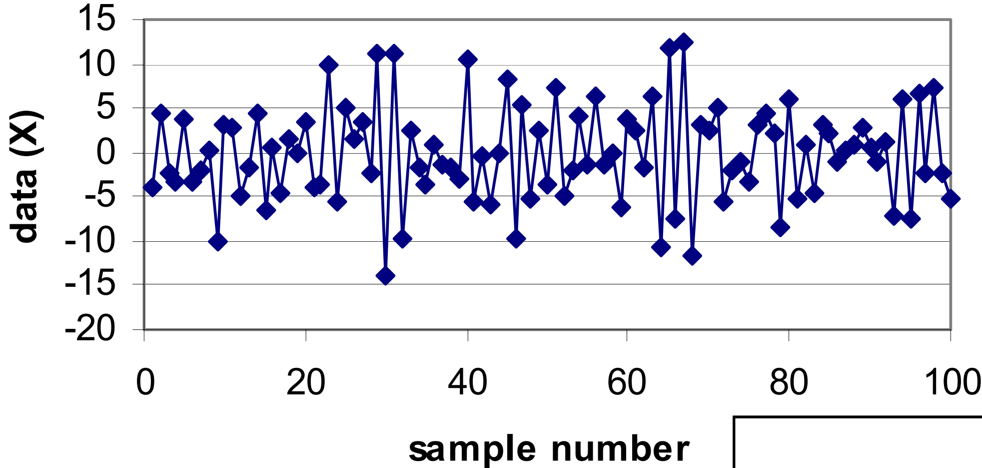
Interpreting Phi



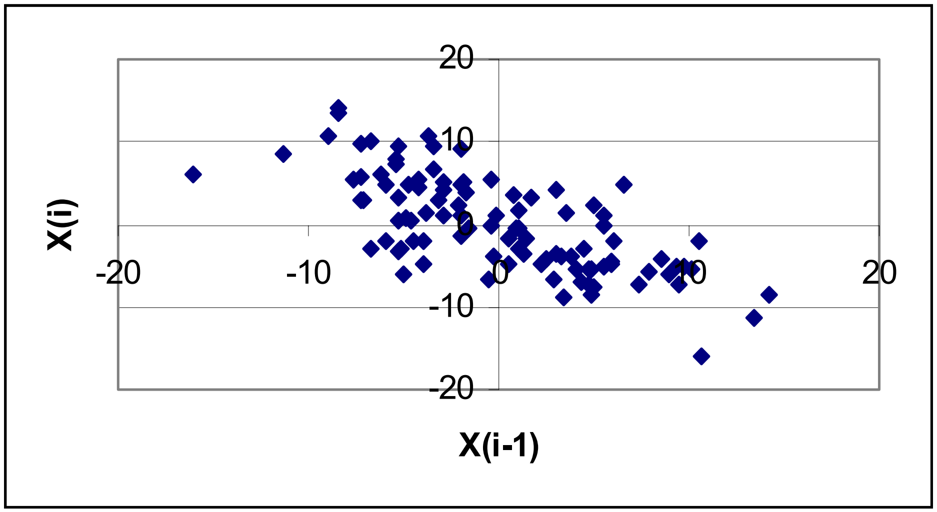
$\phi = 0.9$



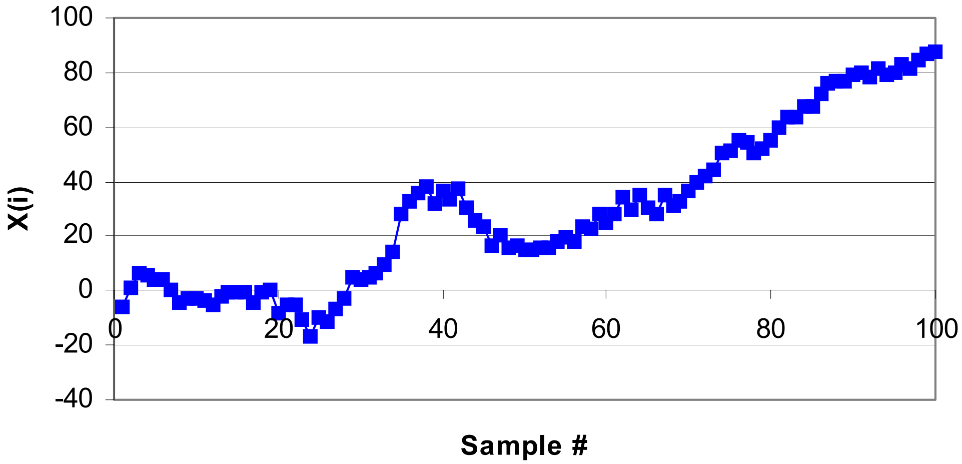
Interpreting Phi



$\phi = -0.7$

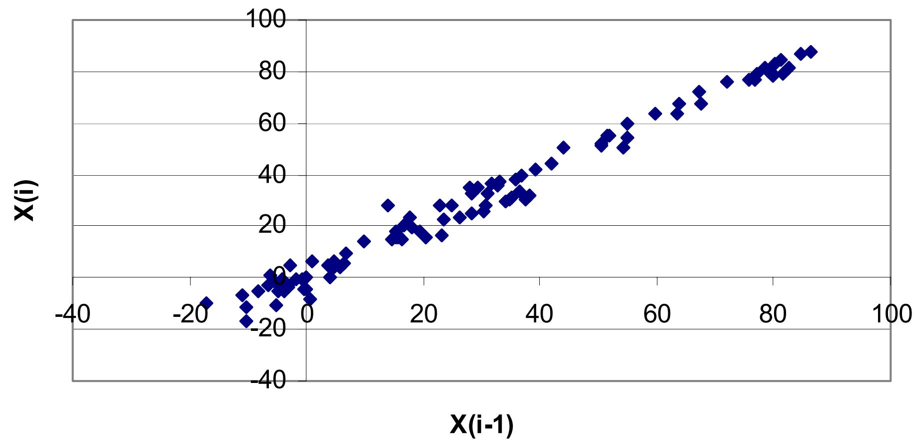


Interpreting Phi



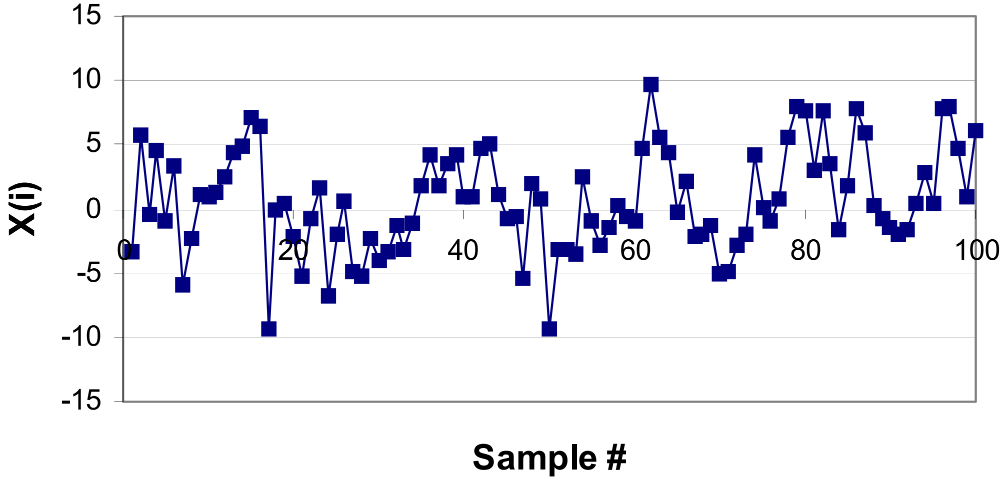
$\phi = 1.02$

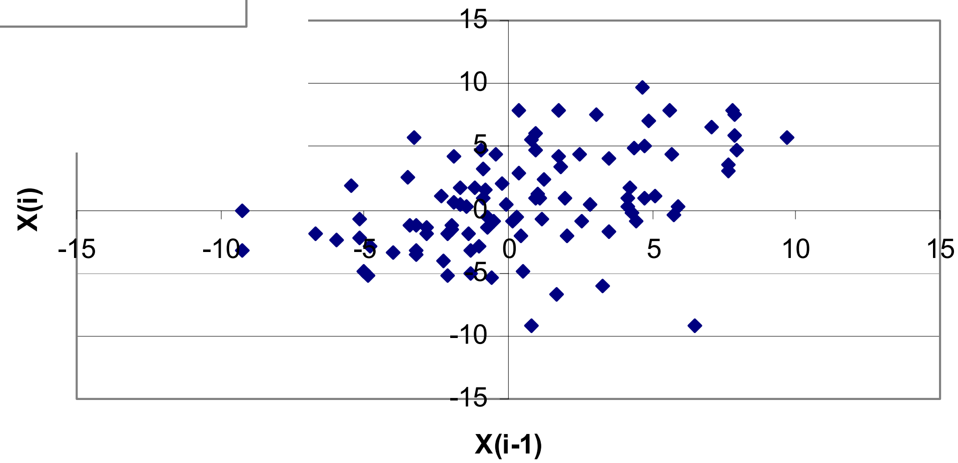
Behavior is unstable because $\phi > 1$



Finding ϕ

Let's say that we have a series of data such as that below





Finding ϕ

Let's apply this model to data: $X_i = \phi X_{i-1} + a_i$

Same form as $y_i = \beta_1 x_i + \varepsilon_i$

We now know how to estimate the value for β_1 (called estimate b_1)

$$S = \sum_{i=1}^{n} (X_i - \hat{X}_i)^2 = \sum_{i=1}^{n} (X_i - \phi X_{i-1})^2$$

$$\frac{dS}{d\phi} = 2\Sigma(X_i - \phi X_{i-1})(-1) = 0$$

Finding ϕ

$$\hat{\phi} = \sum_{i=2}^{n} X_i X_{i-1} \Big/ \sum_{i=2}^{n} X_{i-1}^2$$

For data shown previously,

$$\sum_{i=2}^{n} X_i X_{i-1} = 725.71 \qquad \sum_{i=2}^{n} X_{i-1}^2 = 1562.15$$

$$\hat{\phi} = 0.465$$

So, $\hat{X}_i = \hat{\phi} X_{i-1}$ **-- also can be thought of as a forecast**

Backshift Operator

Define backshift operator as

$$X_{t-1} = BX_t$$

In general,

$$X_{t-j} = B^j X_t$$

Previous equation: $X_i = \phi X_{i-1} + a_i$**, can be rewritten as**

$$X_i = \phi X_{i-1} + a_i \qquad X_i = \phi B X_i + a_i \qquad X_i(1 - \phi B) = a_i$$

$X_i = a_i/(1 - \phi B)$ **-- denominator is characteristic eqn**

More on AR(1)

$X_i = \phi X_{i-1} + a_i$ **, or since** $X_{i-1} = \phi X_{i-2} + a_{i-1}$

$X_i = \phi(\phi X_{i-2} + a_{i-1}) + a_i$ **or** $X_i = \phi^2 X_{i-2} + \phi a_{i-1} + a_i$

or

$X_i = \sum_{j=0}^{k} \phi^j a_{i-j}$ **Note similar form to EWMA**

AR(2) Model

AR(2) model:

$$X_t = \phi_1 X_{t-1} + \phi_2 X_{t-1} + a_t$$

or

$$X_t - \phi_1 X_{t-1} - \phi_2 X_{t-2} = a_t$$

$$a_t \sim \mathrm{NID}\left(0, \sigma_a^2\right)$$