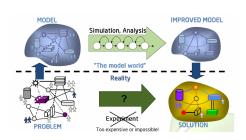
# Modeling & Simulation: Input Data Modelling

Course: Modeling & Simulation - EEN14253

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# What is Input Modeling?

#### What?

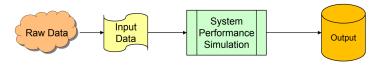
Input modeling for a Discrete Event Simulation (DES) involves analyzing and characterizing real-world data to create accurate probabilistic models that define system inputs.

The different steps for Input Modeling are:

- Data Collection
- Exploratory Data Analysis
- Identification of Suitable Probability Distributions
- Parameter Estimation
- Goodness of Fit
- Verification and Validation

## **Data Collection**

One of the biggest tasks in solving a real problem



- Even when model structure is valid simulation results can be misleading, if the input data is
  - inaccurately collected
  - inappropriately analyzed
  - 3 not representative of the environment
- Inaccurately collected: For example, arrival times at a service desk are recorded manually but with inconsistent timestamps due to human error or forgotten entries, leading to incorrect estimates of the arrival distribution.
- Inappropriately analyzed: Fitting a Normal distribution to highly skewed service time data without testing goodness-of-fit can result in a poor representation of variability, which affects system performance estimates.
- Not representative of the environment: Collecting machine breakdown data during a low-production season and using it to model peak-season operations.

# **Exploratory Data Analysis**

Visualizing and understanding the main characteristics of a dataset before formal modeling

A histogram can be visualized as:

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### Histograms

A histogram is used to display the distribution of data values along the real number line.

- The number of class intervals depends on:
  - The number of observations
  - 2 The dispersion of the data
- Histogram for continuous data corresponds to the probability density function of a theoretical distribution
- Histogram for discrete data corresponds to the probability mass function of a theoretical distribution.
- Same data can be represented with different bin sizes.

# Tools for Identifying the Distribution

•	<b>Scatter Plot</b> :	A scatter dia	agram is a qua	ality tool tha	t can show the	e relationship	between 1	paired data

• Consider two random variables *X* and *Y*. The correlation between these two random variables can be represented as:

• Similarly positive or negative correlation can be represented as:

# Identifying the Distribution

A family of distributions is selected based on:

- The context of the input variable
- Shape of the histogram

The easy to analyze distributions are:

- Exponential
- Normal
- Poisson
- Triangular
- Weibull

Remember the physical characteristics of the process

- Is the process naturally discrete or continuous valued?
  - Is it bounded?
  - Value range?
  - No single and exact distribution for any stochastic input process
  - Goal: obtain a good approximation

# Selecting Family of Distributions

Using physical basis of the distribution as a guide:

- Number of independent events that occur in a fix amount of time or space
- Distribution of a process that is the sum of a number of component processes
- Distribution of a process that is the product of a number of component processes
- Time between independent events or a process time Time between independent events, or a process time that is memoryless
- Time to failure for components
- Modeling uncertainty
- Resamples from actual data collected

# Identifying a Distribution

#### Quantile

A quantile is a cutoff point that divides a probability distribution or dataset into intervals with equal probabilities. Given data is sorted in ascending order:

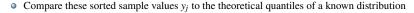
- The 0.25 quantile (also called the 25th percentile or first quartile,  $Q_1$ ) is the value below which 25% of the data falls.
- The 0.5 quantile is the median 50% of the data lies below it.
- The 0.75 quantile (75th percentile or third quartile, Q3) is the value below which 75% of the data lies.

If X is a random variable with a CDF F(x), then the q-quantile of X is a value  $\gamma$  such that

In other words:

Let  $x_i$ , i = 1, 2, 3, ..., n be a sample drawn from the random variable X and  $y_j$ , j = 1, 2, 3, ..., n be the ordered version of this sample in ascending order.

# Q-Q plot to identify a distribution



• For each j-th value, the theoretical quantile is computed as:

where j is the plotting position.

• Using the theoretical quantile, make the Q-Q plot:

• If the data fits the distribution F, the points will lie close to the 45 degree line i.e. slope is 1.

# Q-Q plot to identify a distribution

- ullet Compare these sorted sample values  $y_j$  to the theoretical quantiles of a known distribution
- For each j-th value, the theoretical quantile is computed as:

- where j is the plotting position.
- Using the theoretical quantile, make the Q-Q plot:

• If the data fits the distribution F, the points will lie close to the 45 degree line i.e. slope is 1.

### While evaluating linearity for a Q-Q plot consider:

- The observed values never fall exactly on a straight line
  - The ordered values are ranked and hence not independent, unlikely for the points to be scattered about the line
  - Variance of the extremes is higher than the middle
  - Linearity of the plots in the middle part is more significant

# Q-Q plot to identify a distribution

Ex Consider, the door installation times by a robot collected as

$$T_i = (14.1, 13.7, 14.5, 15.2, 13.9, 14, 15, 14.3, 13.8, 14.6)$$

Using Q-Q plot justify if the above installation times follow an exponential distribution.

## Parameter Estimation for a Distribution

#### Basic Parameters of Importance

Given n observations,  $X_1, X_2, X_3, \ldots, X_n$  (discrete or continuous), the sample mean and variance is given as:

Given a model, the parameters are the actual values which yield a distribution. Typically, from given data, the parameters of a model (i.e. for a distribution) needs to be estimated. Given the standard distributions, the corresponding parameters are:

- Poisson
- Exponential
- Uniform
- Gaussian
- Weibull
- Triangular
- Erlang

## **Estimation of Parameters**

From here onward,  $\theta$  indicates the vector of parameters for any distribution. The two main approaches to estimate parameters of probability distributions are:

- Maximum Likelihood Estimation
- Maximum A Posteriori Estimation

## Maximum Likelihood Estimation

Let  $x_1, x_2, ..., x_n$  be a random sample from a distribution that depends on one or more unknown parameters  $\theta_1, \theta_2, ..., \theta_m$  with probability density (or mass) function  $f(x_i; \theta_1, \theta_2, ..., \theta_m)$ . Then:

#### Likelihood Function

The joint probability density function of  $x_1, x_2, \ldots, x_n$  which is a function of  $\theta_1, \theta_2, \ldots, \theta_n$  is given as:

The above function,  $L(\theta_1, \theta_2, \dots, \theta_m)$  is called the likelihood function.

## Maximum Likelihood Estimation

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#### Maximum Likelihood estimator

If there exists an estimator  $u_1(x_1, x_2, \dots, x_n), \dots, u_m(x_1, x_2, \dots, x_n)$  that maximizes the likelihood function, then

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#### Maximum Likelihood Estimates

The corresponding observed values of the statistics i.e.  $u_1(x_1, x_2, \dots, x_n), \dots, u_m(x_1, x_2, \dots, x_n)$  are called the maximum likelihood estimates of  $\theta_i$ .

## Maximization

The goal in MLE is to use maximization and hence get

•  $\hat{\theta}$  i.e. estimates of the parameter

Using log function properties of monotonicity, we transform the above maximization task as:

#### Thus,

- To develop a MLE, we first express the LF in terms of LLF.
- Choose parameters  $\hat{\theta}$  that maximize the value of LLF.
- To compute maximum first order derivative needs to be computed.

### MLE for Exponential Distribution

Given the PDF of the exponential distribution

$$f(x) = \lambda e^{-\lambda x}$$
 :  $x \ge 0, \lambda > 0$ 

Find the MLE of the exponential distribution parameter  $\lambda$ 

## Maximum Likelihood Estimates

### MLE for Poisson Distribution

Find the MLE of the Poisson distribution parameter  $\lambda$ .

## Maximum Likelihood Estimates

## MLE for Gaussian Distribution

Find the MLE of the Gaussian distribution parameters  $\mu$ ,  $\sigma^2$ .

## Goodness of Fit Tests

Conduct hypothesis testing on input data distribution using

- Kolmogorov-Smirnov test
- Chi-square test

Note there is no single distribution which is correct for input data. Typical mistakes in identifying the correct distribution:

- Type I error
- Type II error

		1			
Statistical	State of the null hypothesis				
Decision	$H_0$ True	$H_0$ False			
		Type II Error			
Accept $H_0$	Correct	Incorrectly accept H <sub>0</sub>			
		False negative			
	Type I Error				
Reject $H_0$	Incorrectly reject H <sub>0</sub>	Correct			
	False positive				

## **Chi-Square Test**

#### Idea

Comparing the histogram of the input data to the shape of the candidate density or mass function.

Valid for large sample sizes when parameters are estimated by maximum-likelihood method. The steps for the Chi-square test are as follows:

- STEP 1: Arrange n observations into k classes. To choose the proper sample size k a guide is given
  as:
  - ① If  $n \le 100$ , k is chosen between 10 to 20
  - 2 If  $n \le 50$ , k is chosen between 5 to 10
  - ③ If  $n \ge 100$ , k is chosen between  $\sqrt{n}$  to n/5
- STEP 2: Estimate the parameters of the distribution using MLE discussed earlier.
- STEP 3: Compute the expected frequency  $E_i$  for each class as:

- STEP 4: Combine categories so that E<sub>i</sub> ≥ 5 for each class. This is mandatory to ensure validity of the Chi-square test.
- STEP 5: Compute the test:

## **Chi-Square Test**

• STEP 6: Get the degrees of freedom as

• STEP 7: Compare with Chi-Square Table or compute p-value to verify hypothesis

The hypothesis for the test is as follows:

- $H_0$ : The data follows the specified distribution (Null Hypothesis)
- $\bullet$   $H_1$ : The data does not follow the specified distribution.

Given a significance value  $\alpha$ ,

if the p-value  $< \alpha$  reject the null hypothesis.

Ex: Given  $\alpha = 0.05$ , check whether the number of calls received per minute at a call center follows a Poisson distribution

Number of calls: 0,1,2,3,4,5 or more

Frequency: 10,26, 35, 25,15,9.

The Chi-square critical values are given as:

df: 1,2,3,4,5,6,7

 $\chi^2(\alpha = 0.05)$ : 3.841, 5.991, 7.815, 9.488, 11.070, 12.592, 14.067

# Selection of Input Models in Absence of Data

If data is not available, some possible sources to obtain information about the process are:

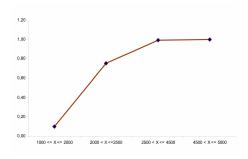
- Engineering data: Often product or process has performance ratings provided by the manufacturer
  or company rules specify time or production standards
- Expert option: People who are experienced with the process or similar processes, often, they can
  provide optimistic, pessimistic and most-likely times, and they may know the variability as well.
- Physical or conventional limitations: physical limits on performance, limits or bounds that narrow the range of the input process.
- The nature of the process

Ex: Example: Production planning simulation.

- Input of sales volume of various products is required, salesperson of product XYZ says that:
  - No fewer than 1000 units and no No fewer than 1000 units and no more than 5000 units will be sold.
  - Given her experience, she believes there is a 90% chance of selling more than 2000 units a 25% more than 2000 units, a 25% chance of selling more than 2500 units, and only a 1% chance of selling more than 4500 units.
- Translating these information into a cumulative probability of being less than or equal to those goals less than or equal to those goals for simulation input

# Selection of Input Models in Absence of Data

i	Interval (Sales)	PDF	Cumulative Frequency, <i>ci</i>
1	$1000 \le X \le 2000$	0.1	0.10
2	$2000 < X \le 2500$	0.65	0.75
3	$2500 < X \le 4500$	0.24	0.99
4	$4500 < X \le 5000$	0.01	1.00



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- However, multiple variables which appear as input may be related

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#### Multivariate Series

A multivariate input model describes the joint behavior of two or more random variables. It captures not just their individual distributions, but also their dependence structure.

- If we are modeling the arrival time and service time in a call center, the random variables can be:
  - 1 Individually distributed: Exponential, Normal, etc.
  - 2 Jointly distributed: Correlated (e.g., busy times = longer service times)

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### Time-Series

A time-series process refers to a sequence of data points or observations that are ordered in time. These observations typically occur at successive, evenly spaced time intervals.

- Stationary Time Series: A stationary process has constant statistical properties over time, such as a constant mean, variance, and autocorrelation.
- Non-Stationary Time Series: A non-stationary time series has properties (e.g., mean or variance) that change over time.

## **Covariance and Correlation**

Consider a bi-variate linear model that describes the relationship between two random variables  $X_1$  and  $X_2$ 

The covariance between the variables can be given as:

Given the values of covariance obtained, the coefficient  $\beta$  can be related as

- If the variables are independent
- If the variables are positively correlated
- If the variables are negatively correlated

The correlation between  $X_1$  and  $X_2$  is given as

## Input Models for Multivariate

For a given two random variables expressed as time-series  $(X_t, X_{t+h})$ ,

- The expression  $cov(X_t, X_{t+h})$  is the lag-h autocovariance.
- The expression  $corr(X_t, X_{t+h})$  is the lag-h autocorrelation.

If the autocovariance value depends only on h and not on t, the time series is *covariance stationary*.

Ex: Let  $X_1$  the average lead time to deliver and  $X_2$  the annual demand for a product, be two random variables given as:

 $X_1 = 6.5, 4.3, 6.9, 6.0, 6.9, 6.9, 5.8, 7.3, 4.5, 6.3$ 

 $X_2 = 103, 83, 116, 97, 112, 104, 106, 109, 92, 96$ 

Find if the variables are correlated.

# Input Models for Time Series

Consider,  $X_1, x_2222, X_3, \ldots$  is a sequence of identically distributed, but dependent and covariance-stationary random variables, then the process can be represented as:

- Autoregressive model of order 1 : AR(1)
- Exponential Autoregressive model of order 1 : **EAR(1)**

Both have the characteristics that

Lag-h autocorrelation decreases geometrically as the lag increases, hence, observations far apart in time are nearly independent.

### Autoregressive Model

It models a variable using its own past values. It assumes that the current value of a time series is linearly dependent on its previous values and a stochastic error term. The generic AR model of order p is represented as:

Consider a time series model represented via a normal distribution as:

# Input Models for Time Series

If the initial value  $X_1$  is chosen appropriately:

•  $X_1, X_2, \dots$  are normally distributed with

The autocorrelation is given as:

The estimates of the parameters are given as: