MEM6810 Engineering Systems Modeling and Simulation 工程系统建模与仿真

Theory Analysis

Lecture 9: Output Analysis II: Comparison

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 - ► Multi-Arm Bandit Problem



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- We now discuss how to compare two or more simulation models, i.e. to estimate their relative performance.
- Here, different simulation models may refer to different designs, operation policies, etc., of a simulated system; in this lecture we simply call them different (system) designs.
- It is one of the most important uses of simulation.



- Key Question: Are the observed differences due to
 - the actual differences on the expected performance of system designs?
 - or the random errors in the simulation outputs?



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 - the actual differences on the expected performance of system designs?
 - or the random errors in the simulation outputs?
- The comparison can be classified into two types:
 - Two system designs: using confidence interval of the difference.
 - Multiple (more than two) system designs: selection of the best.



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	Replication				Sample	Sample
System	1	2		R_i	Mean	Variance
1	Y ₁₁	Y ₂₁		Y_{R_11}	\bar{Y}_1	S_1^2
2	<i>Y</i> ₁₂	Y_{22}	• • •	Y_{R_22}	\bar{Y}_2	S_2^2



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2	Y_{12}	<i>Y</i> ₂₂	• • • •	Y_{R_22}	\bar{Y}_2	S_{2}^{2}

• Point estimator of $\theta_1 - \theta_2$: $\bar{Y}_1 - \bar{Y}_2$.



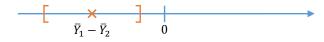
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- Point estimator of $\theta_1 \theta_2$: $\bar{Y}_1 \bar{Y}_2$.
- Approximate 1α CI: $\bar{Y}_1 \bar{Y}_2 \pm t_{v.1-\alpha/2} \times \text{s.e.}(\bar{Y}_1 \bar{Y}_2)$.
 - s.e. $(\bar{Y}_1 \bar{Y}_2)$ is the estimator of standard error of $\bar{Y}_1 \bar{Y}_2$; see more details about this quantity and v later.

[†]The notation here is different from that in Lec 7; the second subscript indicates different system designs. SHEN Haihui

• Case 1 – Strong evidence that $\theta_1 < \theta_2$:

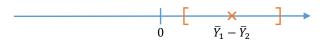




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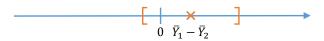
• Case 1 – Strong evidence that $\theta_1 < \theta_2$:



• Case 2 – Strong evidence that $\theta_1 > \theta_2$:



• Case 3 – No strong evidence that one is larger than the other:



• It does not imply $\theta_1 = \theta_2!$



- The first two cases are conclusive.
- If in case 3, then we increase the number of replications R_1 and/or R_2 , after which the CI would likely shift, and definitely shrink in length.

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- If in case 3, then we increase the number of replications R_1 and/or R_2 , after which the CI would likely shift, and definitely shrink in length.
- We will shrink the CI until case 1 or 2 is achieved, or the confidence interval is so narrow, which suggests that we do not need to separate them.



- For the comparison of performance of two designs, there is an important distinction between
 - statistically significant difference (统计意义上的显著区别);
 - practically significant difference (实际意义上的显著区别).



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- Statistical significance answers the following questions:
 - Is the observed difference $ar{Y}_1 ar{Y}_2$ larger than its variability?
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- Practical significance answers the following question:
 - Is the true difference $|\theta_1-\theta_2|$ large enough so it is worthwhile to separate them?



► Significant Difference

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- In case 1, we may reach the conclusion that $\theta_1 < \theta_2$ and decide that design 2 is better (suppose larger is better).
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- However, if the actual difference $|\theta_1 \theta_2|$ is very small, then it might not be worth the cost to replace design 1 with design 2.
- Confidence intervals do not answer the question of practical significance directly.
 - Instead, they bound, with probability $1-\alpha$, the true difference $\theta_1-\theta_2$ within the range $\bar{Y}_1-\bar{Y}_2\pm t_{v,\,1-\alpha/2}\times \mathrm{s.e.}(\bar{Y}_1-\bar{Y}_2)$.
 - Whether a difference within these bounds is practically significant depends on the particular problem.



- Independent sampling means that different random number streams are used to simulate the two systems.
 - All the observations of system 1 $\{Y_{r1}: r=1,\ldots,R_1\}$ are statistically independent of all the observations of system 2 $\{Y_{r2}: r=1,\ldots,R_2\}$.



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- Suppose $Var(Y_{r1}) = \sigma_1^2$ and $Var(Y_{r2}) = \sigma_2^2$. Due to the independence,

$$Var(\bar{Y}_1 - \bar{Y}_2) = Var(\bar{Y}_1) + Var(\bar{Y}_2) = \frac{\sigma_1^2}{R_1} + \frac{\sigma_2^2}{R_2}.$$



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$$S_i^2 = \frac{1}{R_i - 1} \sum_{r=1}^{R_i} (Y_{ri} - \bar{Y}_i)^2.$$



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s.e.
$$(\bar{Y}_1 - \bar{Y}_2) = \sqrt{\frac{S_1^2}{R_1} + \frac{S_2^2}{R_2}}$$
.



• The $1 - \alpha$ CI is approximated by

$$\bar{Y}_1 - \bar{Y}_2 \pm t_{v, 1-\alpha/2} \times \text{s.e.}(\bar{Y}_1 - \bar{Y}_2).$$
 (2)

where s.e. $(\bar{Y}_1 - \bar{Y}_2)$ is given in (1), and the degree of freedom v is

$$v = \frac{[S_1^2/R_1 + S_2^2/R_2]^2}{[S_1^2/R_1]^2/(R_1 - 1) + [S_2^2/R_2]^2/(R_2 - 1)}.$$



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- The approximated CI (2) is called the Welch confidence interval (Welch 1938).
 - ullet Sometimes, people will round v to integer for convenience.



▶ Independent Sampling

• If $R_1=R_2=R$, or we are willing to discard some observations from the system design on which we actually have more data, we can pair Y_{r1} with Y_{r2} to define $Z_r=Y_{r1}-Y_{r2}$, for $r=1,\ldots,R$.



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- Point estimator of $\theta_1 \theta_2$: $\bar{Z} = \frac{1}{R} \sum_{r=1}^R Z_r = \bar{Y}_1 \bar{Y}_2$.

$$\operatorname{Var}(\bar{Z}) = \frac{\operatorname{Var}(Z_r)}{R} = \frac{\operatorname{Var}(Y_{r1} - Y_{r2})}{R} = \frac{\sigma_1^2 + \sigma_2^2}{R}$$
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• To estimate $Var(Z_r)$, instead of estimating σ_1^2 and σ_2^2 separately, we can directly use

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• Approximate $1 - \alpha$ CI:

$$\bar{Z} \pm t_{R-1, 1-\alpha/2} \frac{S}{\sqrt{R}}$$
.



- Common Random Numbers (CRN, also known as correlated sampling): For each replication, the same random numbers are used to simulate both systems.
 - For each replication r, the two estimates, Y_{r1} and Y_{r2} , are correlated.
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- The purpose of using CRN is to induce a positive correlation between Y_{r1} and Y_{r2} for each r and thus to achieve a variance reduction in the point estimator of $\theta_1 \theta_2$, \bar{Z} .

$$Var(\bar{Z}) = \frac{Var(Y_{r1} - Y_{r2})}{R} = \frac{\sigma_1^2 + \sigma_2^2 - 2\rho_{12}\sigma_1\sigma_2}{R}.$$
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- $\mathrm{Var}(\bar{Z})$ in (6) is smaller than that in (3) \Longrightarrow higher precision of point estimator.
- CI is still computed via (4) and (5), but the width will be smaller ⇒ higher precision.

- It is never enough to simply use the same seed for the random-number generator(s):
 - The random numbers must be synchronized: each random number used in one model for some purpose should be used for the same purpose in the other model.
 - E.g., if the ith random number is used to generate a service time at work station 2 for the 5th arrival in model 1, the ith random number should be used for the very same purpose in model 2.



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- The CRN idea is also used when we validate simulation model via input-output transformation, where we prefer to compare the model and actual system under the same historical input, rather than generate the input from input model.



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- Some possible goals:
 - **1** Estimation of each parameter θ_i .
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- The first three can be achieved by simultaneous construction of confidence intervals, whereas the last by some selection approaches.
- From now on, without loss of generality, let's assume the best θ_i is the largest one.

- Assumption 1: For each design i with mean performance θ_i , the noisy output $Y_{ri} \sim \mathcal{N}(\theta_i, \sigma_i^2)$, for $r = 1, 2, \ldots$
- Assumption 2: No CRN is used, i.e., Y_{ri} is independent of Y_{rj} for $i \neq j$.
- Assumption 3 (**indifference-zone**): The gap between the largest θ_i and the second largest θ_i is at least δ , a value known to us.
- Assumption 4 (known variance): σ_i^2 is known, for $i=1,\ldots,k$.



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- Assumption 4 (known variance): σ_i^2 is known, for $i=1,\ldots,k$.
- Bechhofer (1954) first developed a selection procedure, which can ensure the probability of correct selection (PCS):

$$\mathbb{P}\{\text{select the largest } \theta_i\} \ge 1 - \alpha, \tag{7}$$

under Assumptions 1-4, where α is a user specified value and $1-\alpha>1/k$.



- Bechhofer's Procedure
 - \bullet Calculate a constant h, which satisfies

$$\mathbb{P}\{Z_i \le h, \ i = 1, 2, \dots, k - 1\} = 1 - \alpha, \tag{8}$$

where $(Z_1, Z_2, ..., Z_{k-1})^T$ has a multivariate normal distribution with means 0, variances 1, and common pairwise correlations 1/2.

2 For i = 1, ..., k, let

$$n_i = \left\lceil \frac{2h^2\sigma_i^2}{\delta^2} \right\rceil. \tag{9}$$

3 For i = 1, ..., k, run n_i replications for design i and calculate

$$\bar{Y}_i = \frac{1}{n_i} \sum_{r=1}^{n_i} Y_{ri}.$$

4 Select the design with the largest sample mean \bar{Y}_i as the best.



$$\theta_k - \theta_i \ge \delta, \ i = 1, \dots, k - 1. \tag{10}$$



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$$\begin{split} & \mathbb{P}\{\mathsf{select}\ k\} = \mathbb{P}\{\bar{Y}_i - \bar{Y}_k < 0,\ i = 1, \dots, k - 1\} \\ & = \mathbb{P}\left\{\frac{\bar{Y}_i - \bar{Y}_k - (\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}} < \frac{-(\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}},\ i = 1, \dots, k - 1\right\} \\ & = \mathbb{P}\left\{Z_i < \frac{\theta_k - \theta_i}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}},\ i = 1, \dots, k - 1\right\} \end{split}$$



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$$\begin{split} & \mathbb{P}\{\mathsf{select}\;k\} = \mathbb{P}\{\bar{Y}_i - \bar{Y}_k < 0,\; i = 1, \dots, k-1\} \\ & = \mathbb{P}\left\{\frac{\bar{Y}_i - \bar{Y}_k - (\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}} < \frac{-(\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}},\; i = 1, \dots, k-1\right\} \\ & = \mathbb{P}\left\{Z_i < \frac{\theta_k - \theta_i}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}},\; i = 1, \dots, k-1\right\} \\ & \geq \mathbb{P}\left\{Z_i < \frac{\theta_k - \theta_i}{\sqrt{\sigma_k^2/\left(\frac{2h^2\sigma_k^2}{\sigma_k^2}\right) + \sigma_i^2/\left(\frac{2h^2\sigma_i^2}{\sigma_k^2}\right)}},\; i = 1, \dots, k-1\right\} \quad \text{(due to (9))} \end{split}$$



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Proof. (Cont'd)

Now we only need to check that $\mathbf{Z} = (Z_1, Z_2, \dots, Z_{k-1})^\mathsf{T}$ indeed has a multivariate normal distribution with means 0, variances 1, and common pairwise correlations 1/2 (except for some rounding error).



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and $\boldsymbol{Y}=(\bar{Y}_1,\bar{Y}_2,\ldots,\bar{Y}_k)^{\mathsf{T}}$ is a k-variate normal random vector. So, \boldsymbol{Z} , as a linear combination of \boldsymbol{Y} , must be a (k-1)-variate normal random vector.



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Moreover, since $n_i = \left\lceil \frac{2h^2\sigma_i^2}{\delta^2} \right\rceil$ in (9), $\frac{\sigma_i^2}{n_i} = \frac{\delta^2}{2h^2}$ approximately, $i=1,\ldots,k$.



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$$i \neq j$$
, $\operatorname{Cov}(Z_i, Z_j) = \operatorname{Cov}\left(\frac{\bar{Y}_i - \bar{Y}_k}{\delta/h}, \frac{\bar{Y}_j - \bar{Y}_k}{\delta/h}\right) = \frac{\operatorname{Cov}(\bar{Y}_k, \bar{Y}_k)}{\delta^2/h^2} = \frac{\sigma_k^2/n_k}{\delta^2/h^2} = \frac{1}{2}$.



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Hence, by (8) and (11), $\mathbb{P}\{\text{select } k\} \geq 1 - \alpha$.



 Assumption 3 (indifference-zone) can be relaxed by softening the selection target to probability of good selection (PGS):

$$\mathbb{P}\left\{\left|\mathsf{selected}\ \theta_i - \max_{1 \le i \le k} \theta_i\right| < \delta\right\} \ge 1 - \alpha.$$



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- Rinott (1978) proposed a procedure which can still guarantee the PCS in (7) while relaxing Assumption 4 (*known* variance), i.e., allowing *unknown* variances.
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 - It requires an initial stage to estimate σ_i^2 by sample variance.
 - The proof is more complicated.
- Procedures like Bechhofer's or Rinott's are simple to implement, but the efficiency may be low.
 - The designed sample size (or, replication number), n_i , may be larger than necessary (too conservative).



- More sample efficient procedures should be in a sequential manner.
 - Take observations sequentially, i.e., one at a time.
 - Eliminate designs from continued sampling when it is statistically clear that they are inferior.
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 - Simulation for a problem with a single dominant alternative may terminate very quickly.
- Paulson (1964) proposed fully sequential procedures, which can guarantee the PCS in (7), under Assumptions 1-3 and (a) common known variance or (b) common unknown variance.



- Suppose $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_k^2 = \sigma^2$ and σ^2 is known (common known variance).
- Let $\bar{Y}_i(r)$ be the sample mean of the first r observations.



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- Paulson's Procedure
 - **1** Let $0 < \lambda < \delta$ (a good choice is $\lambda = \delta/2$), and

$$a = \ln\left(\frac{k-1}{\alpha}\right) \frac{\sigma^2}{\delta - \lambda}.$$

Let $I = \{1, 2, ..., k\}$ and r = 0.

- 2 Let $r \leftarrow r + 1$. Take one observation from each alternative in I and compute $\bar{Y}_i(r)$, $\forall i \in I$.
- $oxed{3}$ Let $I^{\mathrm{old}}=I$ and

$$I = \left\{\ell \in I^{\mathrm{old}}: \bar{Y}_{\ell}(r) \geq \max_{i \in I^{\mathrm{old}}} \bar{Y}_{i}(r) - \max\{0, a/r - \lambda\}\right\}.$$

If |I| > 1, then go to Step 2; otherwise, select the alternative left in I as the best.

➤ Paulson's Procedure

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- Kim and Nelson (2001) proposed a fully sequential procedure \mathcal{KN} , which extends Paulson's procedure, by allowing *unequal* variances and CRN.
- Commercial simulation software, Simio, implements the \mathcal{KN} procedure of Kim and Nelson (2001) as an Add-In, to help user to select the best scenario.



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 - rank all alternatives
 - select a subset of alternatives
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 - rank all alternatives
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- Existing procedures for R&S (selection of the best) problems:
 - frequentist
 - Bayesian



- Frequentist procedures typically aim to deliver the PCS or PGS; see Kim and Nelson (2006) for a review:
 - two-stage procedures: Bechhofer (1954), Rinott (1978)
 - sequential procedures: Paulson (1964), Kim and Nelson (2001), Hong (2006)



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 - two-stage procedures: Bechhofer (1954), Rinott (1978)
 - sequential procedures: Paulson (1964), Kim and Nelson (2001),
 Hong (2006)
- Bayesian procedures often allocate samples to each alternative either to maximize the Bayesian posterior PCS or to minimize the expected opportunity cost; see Chen et al. (2015) for a review:
 - optimal computing budget allocation: Chen et al. (2000), He et al. (2007)
 - value of information: Chick and Inoue (2001), Chick et al. (2010)
 - knowledge gradient: Frazier et al. (2008), Frazier et al. (2009)
 - economics of selection procedures: Chick and Gans (2009),
 Chick and Frazier (2012)



- Emerging research problems that expend classical R&S from different perspectives; see Hong et al. (2021) for a review:
 - large-scale R&S using parallel computing
 - constrained R&S
 - multi-objective R&S
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- What if the number of candidate designs (feasible solutions) is huge, or countably infinite, or even uncountably infinite?
 - Simulation Optimization (or called Optimization via Simulation)



• R&S Problem vs Multi-Arm Bandit (MAB) Problem:

