MG26018 Simulation Modeling and Analysis
仿真建模与分析

Lecture 8: Output Analysis II: Comparison and Optimization

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Introduction

- We have learnt how to estimate the *absolute performance* of a simulation model.
- 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.

Introduction

- **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?
- 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.

- Let θ_1 and θ_2 be the mean performance of the two system designs in simulation.
- To compare θ_1 and θ_2, we simply construct the point and interval estimates of $\theta_1 - \theta_2$
- Suppose we have the simulation output data from simulation of two system designs.[†]

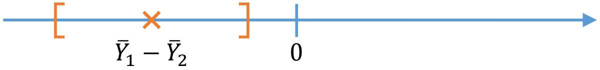
System	*Replication* 1	2	$\cdots$	R_i	*Sample Mean*	*Sample Variance*
1	Y_{11}	Y_{21}	$\cdots$	$Y_{R_1 1}$	$\bar{Y}_1$	S_1^2
2	Y_{12}	Y_{22}	$\cdots$	$Y_{R_2 2}$	$\bar{Y}_2$	S_2^2

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

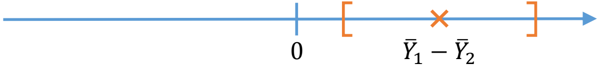
[†] The notation here is different from that in Lec 6; one index here indicates different system designs.

Comparison of Two Designs

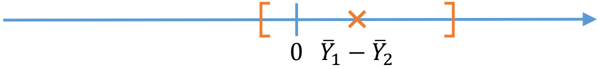
- Case 1 – Strong evidence that $\theta_1 < \theta_2$:



- 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 $\theta_1 = \theta_2$!

Comparison of Two Designs

- 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.
- 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).
- Statistical significance answers the following questions:
  - Is the observed difference $\bar{Y}_1 - \bar{Y}_2$ larger than its variability?
  - Have we collected enough data to be confident that the observed difference is real (not just by chance)?
- Practical significance answers the following question:
  - Is the true difference $|\theta_1 - \theta_2|$ large enough so it is worthwhile to separate them?

- Cases 1 and 2 imply a statistically significant difference, while case 3 does not.
- In case 1, we may reach the conclusion that $\theta_1 < \theta_2$ and decide that design 2 is better (suppose larger is better).
- 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 $\bar{Y}_1 - \bar{Y}_2 \pm t_{v,1-\alpha/2} \times \text{s.e.}(\bar{Y}_1 - \bar{Y}_2)$.
  - 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 $\{Y_{r2} : r = 1, \ldots, R_2\}$.
- Suppose $\mathrm{Var}(Y_{r1}) = \sigma_1^2$ and $\mathrm{Var}(Y_{r2}) = \sigma_2^2$. Due to the independence,

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

  - Standard error of $\bar{Y}_1 - \bar{Y}_2$ is $\sqrt{\frac{\sigma_1^2}{R_1} + \frac{\sigma_2^2}{R_2}}$.
- σ_i^2 is estimated via sample variance

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

  - Standard error of $\bar{Y}_1 - \bar{Y}_2$ is estimated via

$$\mathrm{s.e.}(\bar{Y}_1 - \bar{Y}_2) = \sqrt{\frac{S_1^2}{R_1} + \frac{S_2^2}{R_2}}. \quad (1)$$

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

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

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

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

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

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

$$\begin{aligned} \mathrm{Var}(\bar{Z}) &= \frac{\mathrm{Var}(Z_r)}{R} = \frac{\mathrm{Var}(Y_{r1} - Y_{r2})}{R} = \frac{\sigma_1^2 + \sigma_2^2}{R} \\ &= \mathrm{Var}(\bar{Y}_1 - \bar{Y}_2) = \mathrm{Var}(\bar{Y}_1) + \mathrm{Var}(\bar{Y}_2) = \frac{\sigma_1^2 + \sigma_2^2}{R}. \end{aligned} \tag{3}$$

- To estimate $\mathrm{Var}(Z_r)$, instead of estimating σ_1^2 and σ_2^2 separately, we can directly use

$$S^2 = \frac{1}{R-1}\sum_{r=1}^{R}(Z_r - \bar{Z})^2. \tag{4}$$

- Approximate $1-\alpha$ CI:

$$\bar{Z} \pm t_{R-1,1-\alpha/2}\frac{S}{\sqrt{R}}. \tag{5}$$

- 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.
  - In this case, R_1 and R_2 must be equal, say, $R_1 = R_2 = R$.

- 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 $\theta_1 - \theta_2$, $\bar{Z}$.

$$\mathrm{Var}(\bar{Z}) = \frac{\mathrm{Var}(Y_{r1} - Y_{r2})}{R} = \frac{\sigma_1^2 + \sigma_2^2 - 2\rho_{12}\sigma_1\sigma_2}{R}. \tag{6}$$

- $\mathrm{Var}(\bar{Z})$ in (6) is smaller than that in (3) $\Rightarrow$ higher precision of point estimator.

- CI is still computed via (4) and (5), but the width will be smaller $\Rightarrow$ 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.

- 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.

Comparison of Multiple Designs

- Suppose there are $k > 2$ system designs in total.
- The interested mean performance of design i is θ_i (unknown).
- Some possible goals:
  1. Estimation of each parameter θ_i.
  2. Comparison of each θ_i to a control, say, θ_1 (θ_1 can represent the mean performance of an existing system).
  3. All pairwise comparisons.
  4. Selection of the best θ_i (largest or smallest).
- 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*.

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- 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 $i = 1, \ldots, k$.
- Bechhofer (1954) first developed a selection procedure, which can ensure the probability of correct selection (PCS):
$$\mathbb{P}\{\text{select the largest } \theta_i\} \geq 1 - \alpha, \tag{7}$$
under Assumptions 1-4, where α is a user specified value and $1 - \alpha > 1/k$.

- Bechhofer's Procedure
  1. Calculate a constant h, which satisfies
  $$\mathbb{P}\{Z_i \leq h,\ i = 1, 2, \ldots, k-1\} = 1 - \alpha, \tag{8}$$
  where $(Z_1, Z_2, \ldots, Z_{k-1})^\mathsf{T}$ has a multivariate normal distribution with means 0, variances 1, and common pairwise correlations $1/2$.
  2. For $i = 1, \ldots, k$, let
  $$n_i = \left\lceil \frac{2h^2\sigma_i^2}{\delta^2} \right\rceil. \tag{9}$$
  3. For $i = 1, \ldots, k$, 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.

Proof.

Without loss of generality, assume $\theta_k \geq \theta_{k-1} \geq \cdots \geq \theta_1$. Then Assumption 3 says, $\theta_k - \theta_{k-1} \geq \delta$, which implies that

$$\theta_k - \theta_i \geq \delta, \; i = 1, \ldots, k-1. \tag{10}$$

$$\begin{aligned}
&\mathbb{P}\{\text{select } k\} = \mathbb{P}\{\bar{Y}_i - \bar{Y}_k < 0, \; i = 1, \ldots, k-1\} \\
=&\,\mathbb{P}\left\{ \frac{\bar{Y}_i - \bar{Y}_k - (\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}} < \frac{-(\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}}, \; i = 1, \ldots, k-1 \right\} \\
=&\,\mathbb{P}\left\{ Z_i < \frac{\theta_k - \theta_i}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}}, \; i = 1, \ldots, k-1 \right\} \\
\geq&\,\mathbb{P}\left\{ Z_i < \frac{\theta_k - \theta_i}{\sqrt{\sigma_k^2/(\frac{2h^2\sigma_k^2}{\delta^2}) + \sigma_i^2/(\frac{2h^2\sigma_i^2}{\delta^2})}}, \; i = 1, \ldots, k-1 \right\} \quad \text{(due to (9))} \\
=&\,\mathbb{P}\left\{ Z_i < \frac{\theta_k - \theta_i}{\delta/h}, \; i = 1, \ldots, k-1 \right\} \\
\geq&\,\mathbb{P}\left\{ Z_i < h, \; i = 1, \ldots, k-1 \right\}. \quad \text{(due to (10))}
\end{aligned}$$

Proof. (Cont'd)

Now we only need to check that $\boldsymbol{Z} = (Z_1, Z_2, \ldots, Z_{k-1})^\intercal$ indeed has a multivariate normal distribution with means 0, variances 1, and common pairwise correlations $1/2$.

Recall that

$$Z_i = \frac{\bar{Y}_i - \bar{Y}_k - (\theta_i - \theta_k)}{\sqrt{\sigma_k^2/n_k + \sigma_i^2/n_i}}, \ i = 1, \ldots, k-1,$$

and $\boldsymbol{Y} = (\bar{Y}_1, \bar{Y}_2, \ldots, \bar{Y}_k)^\intercal$ 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.

Besides, $\mathrm{Var}(Z_i) = \frac{\mathrm{Var}(\bar{Y}_i - \bar{Y}_k)}{\sigma_k^2/n_k + \sigma_i^2/n_i} = \frac{\sigma_k^2/n_k + \sigma_i^2/n_i}{\sigma_k^2/n_k + \sigma_i^2/n_i} = 1$.

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, $i = 1, \ldots, k$.

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

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:

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

- Rinott (1978) proposed a procedure which can still guarantee the PCS in (7) while relaxing Assumption 4 (*known* variance), i.e., allowing *unknown* variances.
  - 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.
  - 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.

- Kim and Nelson (2001) proposed a fully sequential procedure $\mathcal{KN}$, which extends Paulson's procedure, by allowing *unequal* variances and CRN.

- 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.
- 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 $I = \{1, 2, \ldots, k\}$ and $r = 0$.
  2. Let $r \leftarrow r + 1$. Take one observation from each alternative in I and compute $\bar{Y}_i(r)$, $\forall i \in I$.
  3. Let $I^{\text{old}} = I$ and
  $$I = \left\{\ell \in I^{\text{old}} : \bar{Y}_\ell(r) \geq \max_{i \in I^{\text{old}}} \bar{Y}_i(r) - \max\{0, a/r - \lambda\}\right\}.$$
  If $|I| > 1$, then go to Step 2; otherwise, select the alternative left in I as the best.

- In Arena, as well as some other simulation softwares like AnyLogic and ProModel, the OptQuest optimization engine is integrated for selecting the best design.
  - OptQuest is based on a combination of methods, including scatter search, tabu search, linear/integer programming, etc.
- Another 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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