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

Theory Analysis

Lecture 7: Output Analysis I: Single Model

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  - The result from a set of simulation runs will be an estimator $\widehat{\theta}$.
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- Types of simulation with regard to output analysis:
  - terminating vs. nonterminating.

- A **terminating simulation** is one that runs for some well-defined time duration T_E.
  - E is a specified event (or set of events) that stops each simulation run (replication).
  - Simulation starts at time 0 under well-specified initial conditions, and ends at the stopping time T_E.
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- Example: A bank opens at 9 AM (*time* 0) with no customers present and 8 of the 11 tellers working (*initial conditions*), and closes at 5 PM (*time $T_E = 8$ hours*).
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- It actually stops service when the last customer who entered before 5 PM has been served.
    - $E = \{$at least 8 hours of simulated time have elapsed and the system is empty$\} \implies T_E$ is a random variable.

- A **nonterminating simulation** is one that runs continuously and without a natural event E to stop the simulation run.
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- For a simulation model that is run in a nonterminating way and *has a steady-state (stationary) distribution*:
  - The objective is often to study the long-run, or steady-state, behavior of a system, which is not influenced by the initial conditions.
  - Such nonterminating simulation is also called *steady-state simulation*.

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- How good is this estimator?
  - Unbiased: $\mathbb{E}[\widehat{\theta}] = \theta$.
  - Consistent: $\widehat{\theta} \xrightarrow{a.s.} \theta$, as $n \to \infty$.[†]

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- Point estimator says *nothing* about the estimation error for finite sample size n.
    - Small estimation error means high estimation precision.

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- σ^2 is typically unknown, and we substitute it by the sample variance

$$S^2 = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \bar{X})^2.$$

- If $X \sim \mathcal{N}(\theta, \sigma^2)$, then

$$\sqrt{n}\left(\frac{\widehat{\theta} - \theta}{S}\right) \sim t_{n-1}, \tag{2}$$

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- Results (2) and (3) are the basis of the confidence interval estimation for θ.

- If $X \sim \mathcal{N}(\theta, \sigma^2)$, where θ and σ are unknown, then a $1 - \alpha$ confidence interval (CI) for θ is

$$\left[\widehat{\theta} - t_{n-1,\, 1-\alpha/2} \frac{S}{\sqrt{n}},\ \widehat{\theta} + t_{n-1,\, 1-\alpha/2} \frac{S}{\sqrt{n}}\right], \qquad (4)$$

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Proof.

$$\mathbb{P} \left\{ \theta \in \left[\widehat{\theta} - t_{n-1,\, 1-\alpha/2} S/\sqrt{n}, \; \widehat{\theta} + t_{n-1,\, 1-\alpha/2} S/\sqrt{n} \right] \right\}$$

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where the last equality is due to (2) and the symmetry of t distribution. ∎

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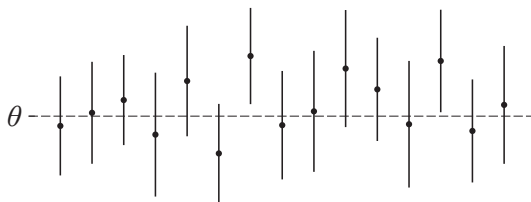
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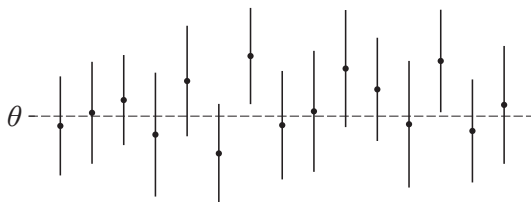
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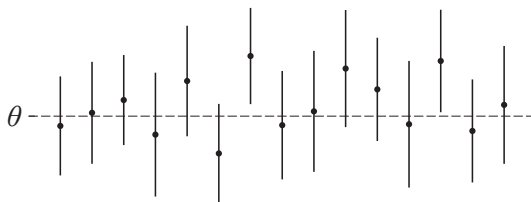 - **Caution**: There is nothing probabilistic about a single CI after the data have been observed and the interval's endpoints have been given numerical values, e.g., $[1.1, \; 2.4]$.

- Try it out! `http://www.rossmanchance.com/applets/ConfSim.html`

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- Take $n^* - n_0$ additional sample points, or start over and take a sample of size n^*, to form the $1 - \alpha$ CI (with new S).

- Suppose an iid sample is taken and the values are as follows:

79.919	3.081	0.062	1.961	5.845	0.941	0.878	3.371	2.157	7.579
3.027	6.505	0.021	0.013	0.123	0.624	5.380	3.148	7.078	23.960
6.769	59.899	1.192	34.760	5.009	0.590	1.928	0.300	0.002	0.543
18.387	0.141	43.565	24.420	0.433	7.004	31.764	1.005	1.147	0.219
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  $n = 50$, $\widehat{\theta} = \bar{X} = 11.894$, $S = 24.953$. We use CI (4) and get
  $t_{49, 0.975} = 2.010$, $t_{49, 0.995} = 2.680$. Then,

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  Take $598 - 50 = 548$ additional sample points.

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- In general, independent replications (runs) are used, each with a different random number stream.

- Within-replication data vs. across-replication data:

Replication	Within-Rep Data (each row)	Across-Rep Data
1	$Y_{11}, Y_{12}, \ldots, Y_{1n_1}$	$\bar{Y}_1 = \frac{1}{n_1} \sum_{i=1}^{n_1} Y_{1i}$
2	$Y_{21}, Y_{22}, \ldots, Y_{2n_2}$	$\bar{Y}_2 = \frac{1}{n_2} \sum_{i=1}^{n_2} Y_{2i}$
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- Use **across-rep** data to do point/interval estimation!

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$$\left[\bar{Y} - t_{R-1,\, 1-\alpha/2} \frac{S}{\sqrt{R}}, \ \bar{Y} + t_{R-1,\, 1-\alpha/2} \frac{S}{\sqrt{R}} \right],$$
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- Necessary number of replications for specified precision $H \le \epsilon$ under $1 - \alpha$ confidence level, can be computed using (6).

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- However, we cannot simulate a system "to infinity" but must stop somewhere.
  - The simulation run length (n or T_E) is a design choice instead of inherently determined by the nature of the problem.

- The run length in steady-state simulation needs to be *carefully chosen*, with several considerations:
    - bias that is due to artificial or arbitrary initial conditions;
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  - budget constraints on the time available to execute the simulation.

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- With more replications, we get a more "precise" estimate of an incorrect value.
  - The confidence interval is narrower but it is centered at an incorrect position.

- Example of $M/M/1$ queue: `https://xiaoweiz.shinyapps.io/MM1queue`
  - If $\lambda < \mu$, the system is stable and the **steady-state expectation** (or **long-run average**) of waiting time is

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} Y_i = \frac{\lambda/\mu}{\mu - \lambda}.$$

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  - Choosing different initial conditions (in this example, number of customers in station, also known as initial state) gives different looks of sample paths (over finite time period).

- Methods to reduce initialization bias:
  - intelligent initialization;
  - warm-up period deletion;
  - low-bias estimator (advanced topic).

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- If the system exists, collect data on it and use these data to specify more nearly typical initial conditions:
  - fit a probability distribution to describe the initial state;
  - or, simply use the sample mean as a representative.

- If the system can be simplified enough to make it analytically solvable, e.g. queueing models, use the theoretical solution to initialize the simulation.
  - Solve the simplified model to find the stationary distribution or most likely conditions (e.g., the expected number of customers in a station).
  - This is another important value of those analytically solvable queueing models.

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  - warm-up period: from time 0 to time T_0;
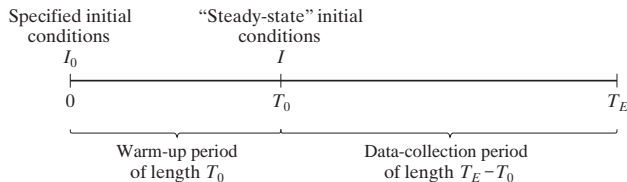 - data-collection period: from time T_0 to T_E.

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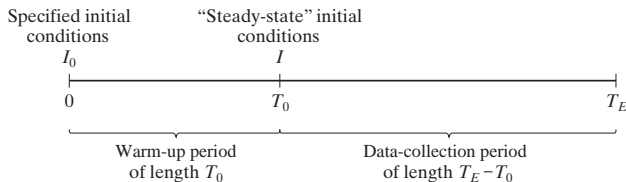 - data-collection period: from time T_0 to T_E.

Figure: Warm-up Period Deletion (*from* Banks et al. (2010))

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Figure: Warm-up Period Deletion (*from* Banks et al. (2010))

- T_0 should be sufficiently large so that at time T_0 the impact of the initial condition is very weak and the system behaves approximately as in the steady state.

- To determine T_0
  - There are no widely accepted and proven techniques.
  - Plots are often used.

- The raw output data plot from a single simulation run is usually too fluctuating to detect the trend. **– not helpful**

- Instead of directly plotting raw output data, we usually use some smoother plots to see when the curve "stabilizes":
  - cumulative average (累积均值); **– OK**
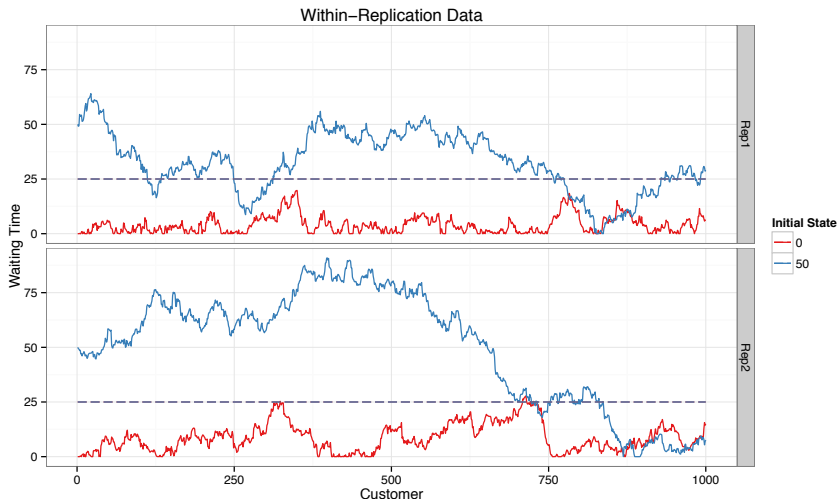 - ensemble average (总体均值). **– recommended**

Figure: Raw Output of Waiting Time of Each Customer in $M/M/1$ Queue with $\lambda = 0.962$ and $\mu = 1$ (from ZHANG Xiaowei)

- Cumulative average (累积均值): For one replication, say, replication 1, plot the average from time 0 up to now.

  - Discrete outputs: Plot $\bar{Y}_1(n) = \frac{1}{n} \sum_{i=1}^{n} Y_{1i}$ with respect to n;

  - Continuous outputs: Plot $\tilde{Y}_1(T) = \frac{1}{T} \int_0^T Y_1(t) \mathrm{d}t$ with respect to T.

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- The cumulative plot is usually conservative, i.e., the warm-up period it detects is longer than necessary.
  - It retains all of the data including the warm-up period, so the bias needs more time to diminish.
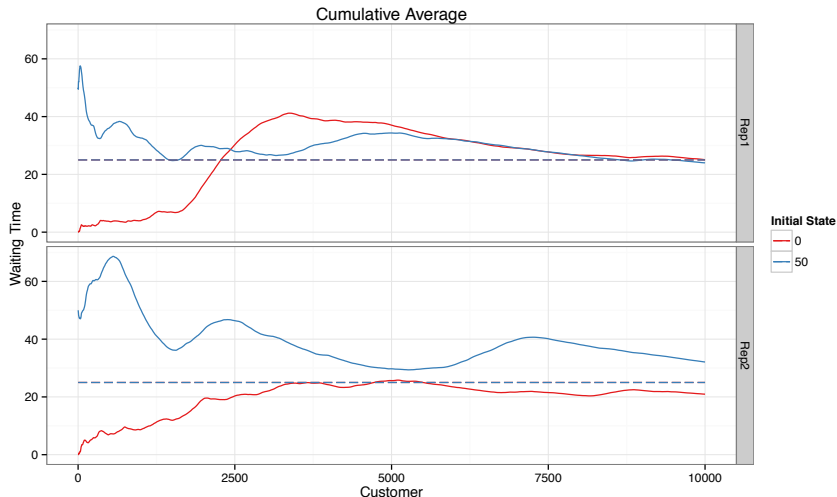
Figure: Cumulative Average Waiting Time of Customers in $M/M/1$ Queue with $\lambda = 0.962$ and $\mu = 1$ (from ZHANG Xiaowei)

- Ensemble average (总体均值): For multiple replications $1, \ldots,$
  R, compute the average across replications and make the plot.
    - Discrete outputs: Plot $\bar{Y}(n) = \frac{1}{R} \sum_{r=1}^{R} Y_{nr}$ with respect to n;
    - Continuous outputs: *Divide the raw data of replication r into small batches*, e.g., $\{Y_r(t) : (j-1)m \le t < jm\}$, $j = 1, 2, \ldots$; plot $\tilde{Y}(j) = \frac{1}{R} \sum_{r=1}^{R} \left[\frac{1}{m} \int_{(j-1)m}^{jm} Y_r(t)\mathrm{d}t \right]$ with respect to j.

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- We detect one warm-up period duration for multiple replications.

- Some variations are smoothed out by averaging across multiple replications.
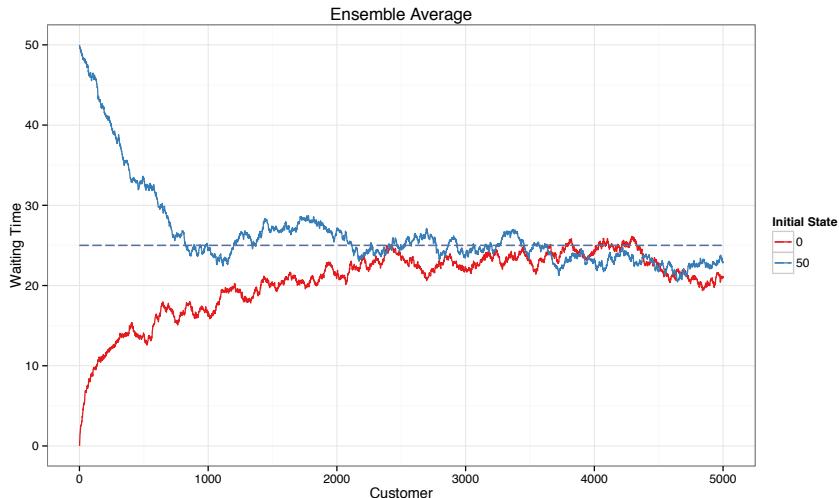 - This leads to more accurate detection of warm-up period.

Figure: Ensemble Average Waiting Time of n-th Customer in $M/M/1$ Queue with $\lambda = 0.962$ and $\mu = 1$ (from ZHANG Xiaowei)

- When first starting to detect the warm-up period, a run length and number of replications will have to be guessed.
  - Increase the number of replications if the ensemble averages are not smooth enough.
  - Increase the run length if the ensemble averages do not stabilize.

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  - Increase the run length if the ensemble averages do not stabilize.

- Since each ensemble average is the sample mean of iid observations across R replications, a confidence interval can be placed around each point.

  - Use them to judge whether or not the plot is precise enough to decide that the bias has vanished.

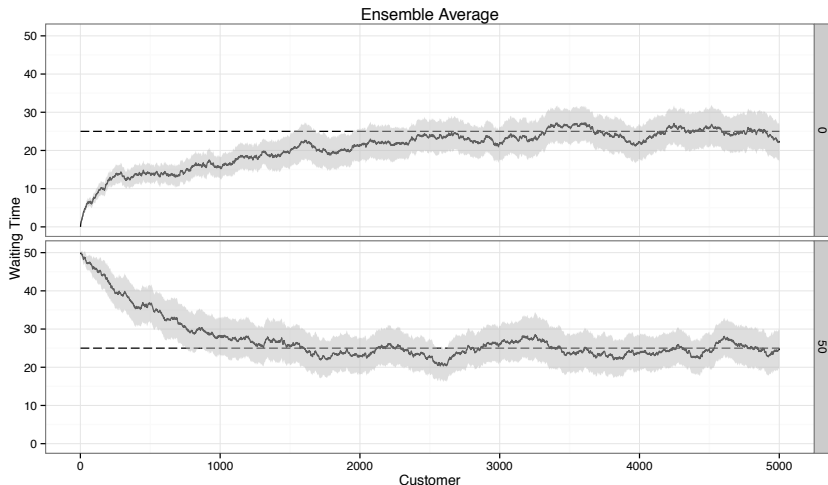 - This is the preferred method to determine a deletion point.

Figure: Ensemble Average Waiting Time and 95% CI of n-th Customer in $M/M/1$ Queue with $\lambda = 0.962$ and $\mu = 1$ (*from ZHANG Xiaowei*)

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- Different performance measures could approach steady state with different speed.

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- Note: Initialization bias is not affected by the number of replications.
  - It is affected by deleting more data (i.e. increasing T_0) or extending the run length (i.e. increasing T_E).
  - Increasing the number of replications could produce narrower interval around the "wrong point".

- Discrete outputs:
    - Suppose we decide to delete first d observations of the total n observations in a replication.[†]
    - The across-replication data from R replications are

$$\bar{Y}_1 = \frac{1}{n-d} \sum_{i=d+1}^{n} Y_{1i} , \ldots, \bar{Y}_R = \frac{1}{n-d} \sum_{i=d+1}^{n} Y_{Ri}.$$

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- Continuous outputs:
  - Suppose we decide to delete data in $[0, T_0]$ period and only use those in $[T_0, T_E]$ in a replication.
  - The across-replication data from R replications are

$$\tilde{Y}_1 = \frac{1}{T_E - T_0} \int_{T_0}^{T_E} Y_1(t)\mathrm{d}t \,,\, \ldots \,,\, \tilde{Y}_R = \frac{1}{T_E - T_0} \int_{T_0}^{T_E} Y_R(t)\mathrm{d}t.$$

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  - So we can use them to compute the point estimator, CI, and necessary number of replications for specified precision, in the same way as before.

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- Unlike terminating simulation, the above mentioned estimators are biased for finite n or T_E.
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- A rough rule for relationship between d and n, or T_0 and T_E:

$$(n - d) \geq 10d, \quad (T_E - T_0) \geq 10T_0.$$

- Suppose analysis indicates that $R - R_0$ additional replications are needed after the initial number R_0, in order to meet the desired precision.

- An alternative to increasing replications is to increase run length T_E within each replication.

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  - Increase run length T_E in the same proportion (R/R_0) to a new run length $(R/R_0)T_E$.

  - More data will be deleted, from time 0 to time $(R/R_0)T_0$.

  - More data will be used to compute the estimate, from time $(R/R_0)T_0$ to time $(R/R_0)T_E$.

  - The total amount of simulation effort is the same as if we had simply increased the number of replications.
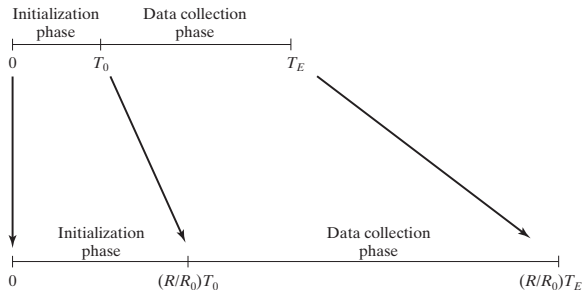
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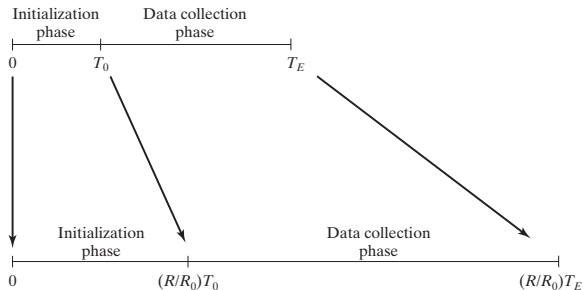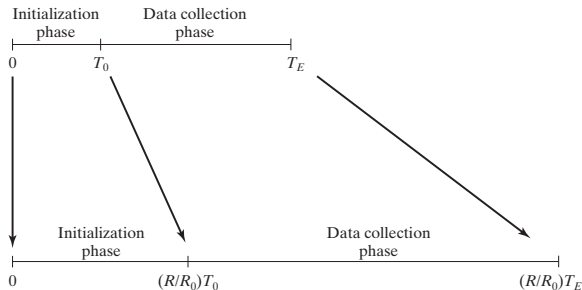
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- Advantage: Any residual bias in the point estimator would be further reduced.

- Disadvantage: It is necessary to have saved the state of the model at time T_E and to be able to continue the running.
  - Otherwise, the simulations would have to be re-run from time 0, which could be time consuming for a complex model.

- A disadvantage of the replication method is that the warm-up period must be deleted on each replication.
  - This can become very costly in terms of computation time especially when the model warms up very slowly.
    - E.g., $M/M/1$ queue with utilization close to 1.

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  - This can become very costly in terms of computation time especially when the model warms up very slowly.
    – E.g., $M/M/1$ queue with utilization close to 1.

- This suggests that we could use one single, (very) long replication for estimation, so that only one warm-up period is deleted.

- Besides, it is also possible that we are in a situation where only the data from one long replication are available.

- Point estimator: Sample mean after the warm-up period deletion

$$\bar{Y} = \frac{1}{n-d} \sum_{i=d+1}^{n} Y_i, \quad \tilde{Y} = \frac{1}{T_E - T_0} \int_{T_0}^{T_E} Y(t)\mathrm{d}t.$$

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- The disadvantage of the single-replication design arises when we try to estimate the variance of the above estimators, because of
  - the strong but unknown dependence among $Y_1, Y_2, \ldots, Y_n$;
  - the non-identical distribution of $Y_1, Y_2, \ldots, Y_n$;
  - and the integral form of $\tilde{Y}$.

- **Caution:** It is tempting to compute

$$S^2 = \frac{1}{n-d-1} \sum_{i=d+1}^{n} (Y_i - \bar{Y})^2,$$

and use $S^2/(n-d)$ to estimate $\mathrm{Var}(\bar{Y})$. However, such estimation will be **terrible**, since $Y_1, Y_2, \ldots, Y_n$ are **neither independent nor identically distributed**.

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- Example: Suppose $Y_{d+1}, \ldots, Y_n$ are identically distributed but positive correlated (which is common for waiting time), then

$$\mathbb{E}[S^2/(n-d)] < \text{Var}(\bar{Y}).$$

  - The constructed CI using $S^2/(n-d)$ will be narrower than the actual valid one.

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$$\underbrace{Y_1, \ldots, Y_d}_{\text{deleted}}, \underbrace{Y_{d+1}, \ldots, Y_{d+m}}_{\text{Batch 1: } \bar{Y}_1}, \underbrace{Y_{d+m+1}, \ldots, Y_{d+2m}}_{\text{Batch 2: } \bar{Y}_2}, \ldots, \underbrace{Y_{d+(k-1)m+1}, \ldots, Y_{d+km}}_{\text{Batch } k: \bar{Y}_k}$$

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- Why it works?
  - The correlation between two observations decreases as they are farther apart.
  - If the batch size is sufficiently large,
    – most of the observations in a batch will be approximately independent of those in other batches;
    – only those near the end of the batches are significantly correlated.

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- However, if the batch size is sufficiently large, successive batch means will be approximately independent.
- Unfortunately, there is no widely accepted and relatively simple method for choosing an acceptable batch size m (or equivalently, choosing a number of batches k).
- Some general guidelines:
  - In most applications, it is suggested to let $10 \leq k \leq 30$, according to Schmeiser (1982).
  - If the run length is to be increased to attain a specified precision, it is suggested to allow both m and k to grow.