# 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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#### Contents

- 1 Introduction
  - ▶ Types of Simulations
- 2 Point and Interval Estimations
  - ▶ Basics
  - ► Specified Precision
  - ► Example
- 3 Terminating Simulation
  - ▶ Discrete Outputs
  - ► Continuous Outputs
- 4 Steady-State Simulation
  - ▶ Initialization Bias
  - ▶ Intelligent Initialization
  - ► Warm-up Period Deletion
  - ► Estimation with Multiple Replications
  - ▶ Estimation with Single Replication



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  - ► Continuous Outputs
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  - Control the estimation precision.
- 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.
  - $E = \{ \text{at least 8 hours of simulated time have elapsed and the system is empty} \} \Longrightarrow T_E \text{ is a random variable.}$

- A nonterminating simulation is one that runs continuously and without a natural event E to stop the simulation run.
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- Examples: Production line that runs 24/7, hospital emergency rooms, continuously operating computer networks, etc.
- 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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  - Consistent:  $\widehat{\theta} \xrightarrow{a.s.} \theta$ , as  $n \to \infty$ .
- Point estimator says *nothing* about the estimation error for finite sample size n.
  - Small estimation error means high estimation precision.



<sup>&</sup>lt;sup>†</sup>Assume  $\mathbb{E}[|X|] < \infty$ , or, a stronger condition,  $\mathrm{Var}(X) < \infty$ .



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- $\sigma^2$  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

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- $\sqrt{n}(\frac{\widehat{\theta}-\theta}{S})\sim\mathcal{N}(0,1)$  approximately when n is large.
- Results (2) and (3) are the basis of the confidence interval estimation for  $\theta$ .





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

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

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



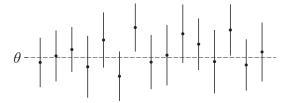


- The interpretation of CI:
  - If one constructs a very large number of independent  $1-\alpha$  Cls, each based on n observations, the proportion of Cls that actually contain (cover)  $\theta$  should be  $1-\alpha$ .



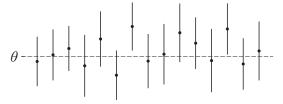


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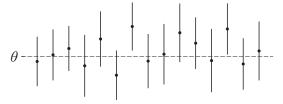


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- Try it out! http://www.rossmanchance.com/applets/ConfSim.html





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• For CI (4), the half-length under  $1-\alpha$  confidence level is

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• Half-length H presents the precision (or error) of the estimation for  $\theta$ .



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$$H = t_{n-1, 1-\alpha/2} \frac{S}{\sqrt{n}}.$$

• For CI (5), the half-length under  $1-\alpha$  confidence level is

$$H = z_{1-\alpha/2} \frac{S}{\sqrt{n}}.$$

- Half-length H presents the precision (or error) of the estimation for  $\theta$ .
- We want H to be small enough for our decision making, say,  $H \leq \epsilon$ , under  $1-\alpha$  confidence level.



Specified Precision

- Usually we take an initial sample of size  $n_0$  to get an estimate of  $\sigma^2$ , say  $S_0^2$ .
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- For Cl (4), an approximate expression for the total sample size required to make  $H \leq \epsilon$  is given by

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- For simplicity, people sometimes use (6), regardless of the distribution of X.
- 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).

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• 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 Cl (4) and get  $t_{49,0.975}=2.010,\ t_{49,0.995}=2.680.$  Then,  $95\%$  Cl:  $11.894\pm2.010\times\frac{24.953}{\sqrt{50}}=11.894\pm7.093=[4.801,18.987];$   $99\%$  Cl:  $11.894\pm2.680\times\frac{24.953}{\sqrt{50}}=11.894\pm9.457=[2.437,21.351].$ 



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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.

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• 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	$Y_{21}, Y_{22}, \ldots, Y_{2n_2}$	$\bar{Y}_2 = \frac{1}{n_2} \sum_{i=1}^{n_2} Y_{2i}$
:	<u>:</u>	:
R	$Y_{R1}, Y_{R2}, \ldots, Y_{Rn_R}$	$\bar{Y}_R = \frac{1}{n_R} \sum_{i=1}^{n_R} Y_{Ri}$



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- Within-rep data are typically neither independent nor identically distributed:
  - waiting times of successive customers are heavily correlated;
  - waiting times during the peak hours are longer than off-peak hours, so they're not identically distributed.
- Use across-rep data to do point/interval estimation!



- Example: What is the expectation of average waiting time for customers during  $[0, T_E]$ ?
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• Necessary number of replications for specified precision  $H \leq \epsilon$  under  $1 - \alpha$  confidence level, can be computed using (6).



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2	$\{Y_2(t): 0 \le t \le T_{E_2}\}$	$\tilde{Y}_2 = \frac{1}{T_{E_2}} \int_0^{T_{E_2}} Y_2(t) dt$
:	<u>:</u>	<u>:</u>
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- Example: What is the expectation of the average waiting line length during  $[0,T_E]$ ?
  - Use  $\{\tilde{Y}_1, \dots, \tilde{Y}_R\}$  as an iid sample of size R, and the rest is similar as before.

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



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  - bias that is due to artificial or arbitrary initial conditions;
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    - measured by the standard error (i.e., estimator's standard deviation) or confidence interval half-width
  - 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.

- ullet 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).



► Intelligent Initialization

 Initialize the simulation in a state that is more representative of long-run conditions.



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  - 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.



► Warm-up Period Deletion

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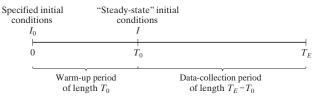


Figure: Warm-up Period Deletion (from Banks et al. (2010))



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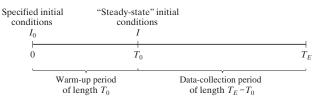


Figure: Warm-up Period Deletion (from Banks et al. (2010))

•  $T_0$  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 <code>ZHANG Xiaowei</code>)

- 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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- It can be plotted for each replication, so we usually detect different warm-up period durations from different replications.
- 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.



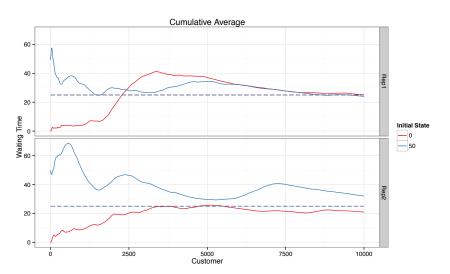


Figure: Cumulative Average Waiting Time of Customers in M/M/1 Queue with  $\lambda=0.962$  and  $\mu=1$  (from ZHANG Xiaowei)

- 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.,  $\{Y_r(t): (j-1)m \leq t < jm\}, \ j=1,2,\ldots;$  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.



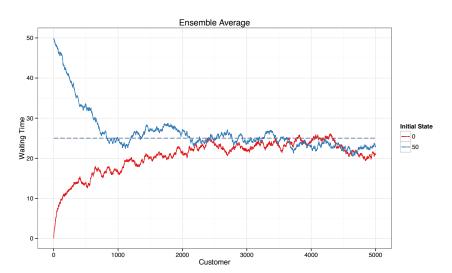


Figure: Ensemble Average Waiting Time of n-th Customer in M/M/1 Queue with  $\lambda=0.962$  and  $\mu=1$  (from ZHANG Xiaowei)



- 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.





- 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.
- 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.



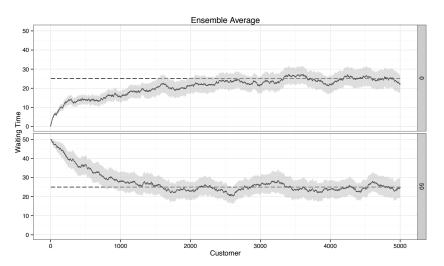


Figure: Ensemble Average Waiting Time and 95% Cl of n-th Customer in M/M/1 Queue with  $\lambda=0.962$  and  $\mu=1$  (from ZHANG Xiaowei)



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

► Estimation with Multiple Replications

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- Idea: Make multiple replications (long enough), remove warm-up period for each one, and then work as if we were in a terminating simulation.
- Caution: Make sure that initialization bias in the point estimator has been reduced to a negligible level.
  - Otherwise the estimation can be misleading.
- 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.<sup>†</sup>
  - ullet The across-replication data from R replications are

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

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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.
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$$\tilde{Y}_1 = \frac{1}{T_E - T_0} \int_{T_0}^{T_E} Y_1(t) dt$$
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- Unlike terminating simulation, the above mentioned estimators are biased for finite n or  $T_E$ .
  - The bias is negligible if d and n, or  $T_0$  and  $T_E$ , are sufficiently large.
- A rough rule for relationship between d and n, or  $T_0$  and  $T_E$ :

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



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



## ► Estimation with Multiple Replications

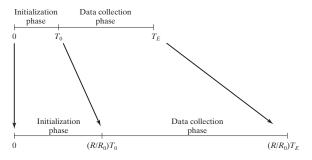


Figure: Increasing Run Length to Achieve Specified Precision (from Banks et al. (2010))



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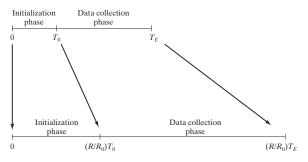


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 Advantage: Any residual bias in the point estimator would be further reduced.



# Steady-State Simulation ► Estimation with Multiple Replications

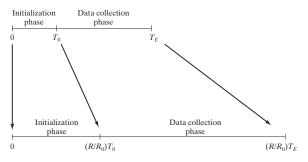


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- Advantage: Any residual bias in the point estimator would be further reduced.
- Disadvantage: It is necessary to have saved the state of the model at time  $T_E$  and to be able to continue the running.
  - Otherwise, the simulations would have to be re-run from time 0, which could be time consuming for a complex model.

SHEN Haihui

- 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.



- 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.
- 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

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



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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  $Y_1, Y_2, \dots, Y_n$ ;
  - the non-identical distribution of  $Y_1, Y_2, \ldots, Y_n$ ;
  - and the integral form of  $\tilde{Y}$ .



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

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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• 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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- Treat the means of these batches as if they were independent.
- 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.

► Estimation with Single Replication

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- Some general guidelines:
  - In most applications, it is suggested to let  $10 \le k \le 30$ , 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.

