Chapter 8: Statistical Analysis of Simulated Data With Confidence Intervals for the Variance

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## Outline

8.1 The Sample Mean and Sample Variance
8.2 Interval Estimates of a Population Mean
8.2½ Confidence Intervals for the Variance
8.3 The Bootstrapping Technique for Estimating the Mean Square Error

Homework

### 8.1 The Sample Mean and Sample Vairince

Suppose we have $X_{1}, \ldots, X_{n}$ independent and identically distributed all from $f(X)$. Let $\theta=E\left[X_{i}\right]$ and $\sigma^{2}=\operatorname{var}\left[X_{i}\right]$, i.e. same mean and variance.

With the arithmetic mean being $\bar{X}=\sum_{i=1}^{n} \frac{X_{i}}{n}$,
we know that $E[\bar{X}]=E\left[\sum_{i=1}^{n} \frac{X_{i}}{n}\right]$

$$
=\sum_{i=1}^{n} \frac{E\left[X_{i}\right]}{n}
$$

$$
=\quad \frac{n \theta}{n}=\theta
$$

### 8.1 The Sample Mean and Sample Variance

If the expected value of a statistic is equal to the parameter it is estimating, it is said to be an unbiased estimator.

To determine the "worth" of $\bar{X}$ an estimator for $\theta$, We look at expected squared difference.

$$
\begin{aligned}
E\left[(\bar{X}-\theta)^{2}\right] & =\operatorname{var}(\bar{X}) \\
& =\operatorname{var}\left(\frac{1}{n} \sum_{i=1}^{n} X_{i}\right) \\
& =\frac{1}{n^{2}} \sum_{i=1}^{n} \operatorname{var}\left(X_{i}\right) \\
& =\frac{\sigma^{2}}{n}
\end{aligned}
$$

### 8.1 The Sample Mean and Sample Vairince

By Chebyshev's inequality
$P\left\{|\bar{X}-\theta|>\frac{c \sigma}{\sqrt{n}}\right\} \leq \frac{1}{c^{2}}$
But using the Central Limit Theorem when $n$ is large, $P\left\{|\bar{X}-\theta|>\frac{c \sigma}{\sqrt{n}}\right\}=P\{|Z|>c\}=2[1-\Phi(c)]$

$$
\begin{aligned}
c & =1.96 \\
P\} & =\frac{1}{(1.96)^{2}}=.2603
\end{aligned}
$$

where $\Phi$ is the cumulative distribution function of the standard normal distribution.

### 8.1 The Sample Mean and Sample Vairince

If we define $S^{2}$ to be
$S^{2}=\frac{1}{n-1} \sum_{i=1}^{n}\left(X_{i}-\bar{X}\right)^{2}$,
we know that it is unbiased because

$$
\frac{(n-1) S^{2}}{\sigma^{2}} \sim \chi^{2}(n-1)
$$

and because the mean of a $\chi^{2}$ is $d f=(n-1)$, therefore

$$
E\left[\frac{(n-1) S^{2}}{\sigma^{2}}\right]=n-1 \longrightarrow \frac{(n-1)}{\sigma^{2}} E\left[S^{2}\right]=n-1 \longrightarrow E\left[S^{2}\right]=\sigma^{2}
$$

### 8.1 The Sample Mean and Sample Vairince

In a simulation, we often generate an extremely large
number of random variates (i.e. $10^{6}$ ).
It would be great if we knew when we had enough.

Assume that we are interested in estimating the value of $\theta=E\left[X_{i}\right]$. One stopping rule is to specify a standard deviation $d$ for $\bar{X}$.

Then, continue generating random variates until $S / \sqrt{n}<d$.
When $n$ is small the following is recommended.

### 8.1 The Sample Mean and Sample Variance

## Method for Determining When to Stop Generating New Data

1. Choose an acceptable value of $d$ for the standard deviation of the estimator.
2. Generate at least 100 data values.
3. Continue to generate additional data values, stopping when you have generated $k$ values and $S / \sqrt{k}<d$, where $S$ is the sample standard deviation based on those $k$ values.
4. The estimate of $\theta$ is given by $\bar{X}=\frac{1}{k} \sum_{i=1}^{k} X_{i}$.

### 8.2 Interval Estimates of a Population Mean

Assume we have $X_{1}, \ldots, X_{n}$ iid all from the same distribution $f(X)$. We use $\bar{X}$ as a "point" estimator for the population mean $\theta$.

We can also generate an "interval" estimator for $\theta$.
We know that $E[\bar{X}]=\theta$ and $\operatorname{Var}[\bar{X}]=\frac{\sigma^{2}}{n}$.
We use the fact that when $n$ is large, $\bar{X}$ has an approximate normal distribution, i.e. $\bar{X} \dot{\sim} N\left(\theta, \sigma^{2} / n\right)$.

### 8.2 Interval Estimates of a Population Mean

What this implies is that $z=\frac{\bar{X}-\theta}{\sigma / \sqrt{n}}$
has an approximate standard deviation!
$P(-1.96<z<1.96)=0.95$
or more generally, $P\left(-z_{\frac{\alpha}{2}}<z<z_{\frac{\alpha}{2}}\right)=1-\alpha$.


## MSSC 6020 Statistical Simulation

### 8.2 Interval Estimates of a Population Mean

The inequality


$$
\begin{array}{rcc}
-z_{\frac{\alpha}{2}} & < & z \\
-z_{\frac{\alpha}{2}} & <\frac{\bar{X}-\mu_{\bar{x}}}{\sigma_{\bar{x}}} \\
-z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}} & <\bar{X}-\mu \\
-z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}-\bar{X} & < & -\mu \\
\bar{X}+z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}} & > & \mu
\end{array}
$$

### 8.2 Interval Estimates of a Population Mean

The inequality

$$
\begin{aligned}
& P\left(-z_{\frac{\alpha}{2}}<z<z_{\frac{\alpha}{2}}\right)=1-\alpha \\
& \frac{\bar{X}-\mu_{\bar{x}}}{\sigma_{\bar{x}}}<\quad z_{\frac{\alpha}{2}} \\
& \bar{X}-\mu<z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}} \\
& -\mu<z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}-\bar{X} \\
& \mu>\bar{X}-z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}
\end{aligned}
$$

### 8.2 Interval Estimates of a Population Mean

We can see the equivalency of these statements

$$
P\left(-z_{\frac{\alpha}{2}}<z<z_{\frac{\alpha}{2}}\right)=1-\alpha \rightarrow P\left\{\bar{X}-z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}<\mu<\bar{X}+z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}\right\}=1-\alpha
$$

Thus a $(1-\alpha) \times 100 \%$ confidence interval for $\theta$ is

$$
\bar{X}-z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}<\mu<\bar{X}+z_{\frac{\alpha}{2}} \frac{\sigma}{\sqrt{n}}
$$

which if $\alpha=0.05$, a $95 \%$ confidence interval for $\theta$ is

$$
\bar{X}-1.96 \frac{\sigma}{\sqrt{n}}<\mu<\bar{X}+1.96 \frac{\sigma}{\sqrt{n}} .
$$

### 8.2 Interval Estimates of a Population Mean

Using similar logic, it is also true that when $\sigma$ is unknown, a (1- $\alpha) \times 100 \%$ confidence interval for $\theta$ is

$$
\bar{X}-t_{\frac{\alpha}{2}, n-1} \frac{s}{\sqrt{n}}<\mu<\bar{X}+t_{\frac{\alpha}{2}, n-1} \frac{s}{\sqrt{n}}
$$

$$
t=
$$

and if $n$ is large,

$$
\bar{X}-z_{\frac{\alpha}{2}} \frac{s}{\sqrt{n}}<\mu<\bar{X}+z_{\frac{\alpha}{2}} \frac{s}{\sqrt{n}}
$$

which if $\alpha=0.05$, a 95\% confidence interval for $\theta$ is

$$
\bar{X}-1.96 \frac{s}{\sqrt{n}}<\mu<\bar{X}+1.96 \frac{s}{\sqrt{n}} .
$$

### 8.2 Interval Estimates of a Population Mean

For Bernoulli random variates, where

$$
X_{i}=\left\{\begin{array}{l}
1 \text { with probability } \quad p \\
0 \text { with probability } 1-p
\end{array}\right.
$$

## Central Limit Theorem

$$
\text { Think of } \bar{X}=\frac{1}{n} \sum_{i=1}^{n} X_{i},
$$

$$
\begin{aligned}
\bar{X} & \sim N\left(\mu, \sigma^{2} / n\right) \text { as } n \rightarrow \infty \\
\mu & =n p \quad \sigma^{2}=n p(1-p)
\end{aligned}
$$

we have the same scenario. Using similar logic,
a $(1-\alpha) \times 100 \%$ confidence interval for $p$ is

$$
P\left\{\bar{X}-z_{\frac{\alpha}{2}} \sqrt{\frac{\bar{X}(1-\bar{X})}{n}}<p<\bar{X}+z_{\frac{\alpha}{2}} \sqrt{\frac{\bar{X}(1-\bar{X})}{n}}\right\}=1-\alpha
$$

$\bar{X}$ is the average of Bernoulli random variables
when $\boldsymbol{n}$ is large.

## 8.2½ Confidence Intervals for the Variance

We know that if $x_{1}, \ldots, x_{n}$ are iid $N\left(\mu, \sigma^{2}\right)$ then the distribution of $\frac{(n-1) s^{2}}{\sigma^{2}}$ is a $\chi^{2}$ with $n$ - 1 degrees of freedom.
A $\chi^{2}$ distribution with $n-1$ degrees of freedom has a mean of $n-1$ and a variance of $2(n-1)$.

This means that the mean and variance of $s^{2}$ are $\sigma^{2}$ and $\frac{2 \sigma^{4}}{(n-1)}$ !

$$
E\left(s^{2}\right)=\sigma^{2} \quad \operatorname{var}\left(s^{2}\right)=\frac{2 \sigma^{4}}{(n-1)}
$$

## 8.2½ Confidence Intervals for the Variance

Following the general $P E \pm C V \times S E(P E)$ procedure, the confidence interval for the variance should be

$$
s^{2} \pm \chi^{2}\left(\frac{\alpha}{2}\right) \sqrt{\frac{2 \sigma^{4}}{n-1}} ?
$$

This is what you were taught in your first stats class.

Is this correct even though the $\chi^{2}$ distribution is not symmetric?

The answer is no.

## 8.2½ Confidence Intervals for the Variance

We know $x=\frac{(n-1) s^{2}}{\sigma^{2}}$ has a chi-square PDF with ( $n-1$ ) degrees of freedom

$$
\begin{gathered}
f(x \mid v)=\frac{x^{v / 2-1} e^{-x / 2}}{\Gamma(v / 2) 2^{v / 2}} \\
E(x \mid v)=v \\
\operatorname{var}(x \mid v)=2 v
\end{gathered}
$$



## 8.2½ Confidence Intervals for the Variance

So we should be able to find $a$ and $b$ such that

$$
\begin{aligned}
& P\left\{a<\frac{(n-1) s^{2}}{\sigma^{2}}<b\right\}=1-\alpha \\
& \int_{0}^{a} f(x) d x=\frac{\alpha}{2} \\
& \int_{0}^{b} f(x) d x=1-\frac{\alpha}{2}
\end{aligned}
$$



## 8.2½ Confidence Intervals for the Variance

Once we have $a$ and $b$, we can look at

$$
P\left\{a<\frac{(n-1) s^{2}}{\sigma^{2}}<b\right\}=1-\alpha
$$

then do a little algebra to get

$$
P\left\{\frac{(n-1) s^{2}}{b}<\sigma^{2}<\frac{(n-1) s^{2}}{a}\right\}=1-\alpha .
$$



## 8.2½ Confidence Intervals for the Variance

So $\frac{(n-1) s^{2}}{b}<\sigma^{2}<\frac{(n-1) s^{2}}{a}$
is a $100(1-\alpha) \%$ confidence interval for $\sigma^{2}$.
$a=1.6899, b=16.0128$
$L=0.0625 s^{2}, U=0.5918 s^{2}$
$U-L=0.5293 s^{2}$


## 8.2½ Confidence Intervals for the Variance

But this confidence interval

$$
\frac{(n-1) s^{2}}{b}<\sigma^{2}<\frac{(n-1) s^{2}}{a}
$$

is not best!
We can find a minimum length confidence interval for $\sigma^{2}$ where the probability in each tail is not equal.

$$
\frac{(n-1) s^{2}}{d}<\sigma^{2}<\frac{(n-1) s^{2}}{c}
$$



## 8.2½ Confidence Intervals for the Variance

So the goal is to minimize

$$
\frac{(n-1) s^{2}}{d}<\sigma^{2}<\frac{(n-1) s^{2}}{c}
$$

subject to the constraint
that $\int_{c}^{d} f(x) d x=1-\alpha$.
Some amount $\alpha_{L}$ in lower tail and some amount $\alpha_{U}$ in upper tail.
$\alpha_{L}+\alpha_{U}=\alpha$


## 8.2½ Confidence Intervals for the Variance

$$
\frac{(n-1) s^{2}}{d}<\sigma^{2}<\frac{(n-1) s^{2}}{c}
$$

In terms of a cost/score function,

$$
\phi=\left(\frac{1}{c}-\frac{1}{d}\right)(n-1) s^{2}+\lambda\left(\int_{c}^{d} f(x) d x-1+\alpha\right)
$$

where $\lambda$ is the Lagrange multiplier.
$a=1.6899, b=16.0128$
$L=0.0625(n-1) s^{2}, U=0.5918(n-1) s^{2}$
$U-L=0.5293(n-1) s^{2}$
$c=2.1473, d=23.7944$
$L=0.0420(n-1) s^{2}, U=0.4657(n-1) s^{2}$
$U-L=0.4237(n-1) s^{2}$.


### 8.3 The Bootstrapping Technique for Estimating Mean Squares

Assume that $X_{1}, \ldots, X_{n}$ are independent and identically distributed from cumulative distribution function $F$.

If $\theta$ is a parameter of interested and $g\left(X_{1}, \ldots, X_{n}\right)$ an estimator, we would like to estimate the value of

$$
\operatorname{MSE}(F)=E_{F}\left[\left(g\left(X_{1}, \ldots, X_{n}\right)-\theta(F)\right)^{2}\right]
$$

we can usually estimate it analytically if $F$ is known

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

But when $F$ is not known, all we have is $X_{1}, \ldots, X_{n}$.

As we know we can estimate $F$ by the empirical CDF

$$
F_{e}(x)=\frac{\text { number of } i: X_{i} \leq x}{n}
$$

$F_{e}$ should be "close" to $F$ especially if $n$ is large and
$F_{e}$ converges to $F$ as $n \rightarrow \infty$.

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

Let's examine the bootstrap approximation to the MSE. when we don't need it. Assume $\theta=\mu$ and $g\left(X_{1}, \ldots, X_{n}\right)=\bar{X}$.

Then we know that $M S E=E\left[(\bar{X}-\mu)^{2}\right]=\sigma^{2} / n$, which we would estimate by $S^{2} / n$.

To estimate the MSE via bootstrap, we have to calculate $\operatorname{MSE}\left(F_{e}\right)=E_{F_{e}}\left[\left(g\left(X_{1}, \ldots, X_{n}\right)-\theta\left(F_{e}\right)\right)^{2}\right]$

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

If we think of $X_{1}, \ldots, X_{n}$ as a population of values, then the vector ( $x_{1}, \ldots, x_{n}$ ), where each element is drawn from
$X_{1}, \ldots, X_{n}$ with replacement can take on $n^{n}$ possible values.

The MSE is then approximately

$$
\operatorname{MSE}\left(F_{e}\right)=\sum_{i_{n}} \cdots \sum_{i_{1}} \frac{\left[\left(g\left(X_{i_{i}}, \ldots, X_{i_{n}}\right)-\theta\left(F_{e}\right)\right)^{2}\right]}{n^{n}} \quad i_{j} \in\{1, \ldots, n\}, j=1, \ldots, n
$$

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

The MSE is approximately

$$
\operatorname{MSE}\left(F_{e}\right)=\sum_{i_{n}} \cdots \sum_{i_{1}} \frac{\left[\left(g\left(X_{i_{1}}, \ldots, X_{i_{i}}\right)-\theta\left(F_{e}\right)\right)^{2}\right]}{n^{n}} \quad i_{j} \in\{1, \ldots, n\}, j=1, \ldots, n
$$

But this requires summing $n^{n}$ terms, a daunting task.
If $n=20$, then there are $1.0486 \times 10^{26}$ terms!

To get around this, we use simulation and approximate the empirical MSE.

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

From $X_{1}, \ldots, X_{n}$, generate $r$ samples of size $n$ with replacement

$$
\begin{aligned}
& X_{1}^{(1)}, \ldots, X_{n}^{(1)} Y_{1}=\left[\left(g\left(X_{1}^{(1)}, \ldots, X_{n}^{(1)}\right)-\theta\left(F_{e}\right)\right]^{2}\right. \\
& X_{1}^{(2)}, \ldots, X_{n}^{(2)} \longrightarrow \\
& \vdots Y_{2}=\left[\left(g\left(X_{1}^{(2)}, \ldots, X_{n}^{(2)}\right)-\theta\left(F_{e}\right)\right]^{2}\right. \\
& \vdots \\
& X_{1}^{(r)}, \ldots, X_{n}^{(r)} \\
& \\
& Y_{r}=\left[\left(g\left(X_{1}^{(r)}, \ldots, X_{n}^{(r)}\right)-\theta\left(F_{e}\right)\right]^{2}\right. \\
& Y_{1}, Y_{2}, \ldots, Y_{r} \longrightarrow \\
& M S E\left(F_{e}\right) \approx \frac{1}{r} \sum_{i=1}^{r} Y_{i}
\end{aligned}
$$

### 8.3 The Bootstrapping Technique for Estimating Mean Squares

From $X_{1}, \ldots, X_{n}$, generate $r$ samples of size $n$ with replacement

$$
\begin{array}{rlrl}
X_{1}^{(1)}, \ldots, X_{n}^{(1)} \\
X_{1}^{(2)}, \ldots, X_{n}^{(2)} & \longrightarrow & Y_{1} & =\left[s_{(1)}^{2}-s^{2}\left(X_{1}, \ldots, X_{n}\right)\right]^{2} \\
\vdots & Y_{2} & =\left[s_{(2)}^{2}-s^{2}\left(X_{1}, \ldots, X_{n}\right)\right]^{2} \\
& \vdots \\
X_{1}^{(r)}, \ldots, X_{n}^{(r)} & & Y_{r} & =\left[s_{(r)}^{2}-s^{2}\left(X_{1}, \ldots, X_{n}\right)\right]^{2} \\
& & \\
Y_{1}, Y_{2}, \ldots, Y_{r} & \longrightarrow & \operatorname{MSE}\left(s_{F e}^{2}\right) \approx \frac{1}{r} \sum_{i=1}^{r} Y_{i}
\end{array}
$$

MSSC 6020 Statistical Simulation Discussion

## Questions?

1. Generate $10^{6}$ sets of 8 random data values from a normal $\mu=100, \sigma=3$. Calculate $s^{2}$ for each.
Make a histogram and form eCDF. Compare the eCDF percentiles to the theoretical percentiles.
2. Find the $4 \%$ minimum length CI for $\sigma^{2}$ when we have $v=7$. Compare the min length Confidence Interval values to the usual $2 \%$ in each tail. Generically assume $s^{2}=1$. Comment.

## Homework 10

$$
E[\bar{x}]=\mu \quad E\left[s^{2}\right]=\sigma^{2}
$$

$\operatorname{var}[\bar{x}]=\frac{\sigma^{2}}{n} \quad \operatorname{var}\left[s^{2}\right]=\frac{2 \sigma^{4}}{n-1}$
3. Generate $n=25$ random numbers from a normal distribution with $\mu=100$ and $\sigma=5$. Compute $\bar{x}$ and $s^{2}$. Generate $m=10^{5}$ bootstrap samples of size $n=25$ from your sample.
a) Compute the mean and variance of each sample.
b) Make a histograms of means and variances in a).
c) Compute mean and variance of means and variances in a).
d) Compute bootstrap estimate of $\operatorname{var}\left(s^{2}\right)$.
e) Compare theoretical values to bootstrap values.
g) Repeat with larger/smaller $n$.
h) Comment.

