Statistical Simulation

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Overview

- Definition of Statistical Simulation
- 2 Problems can be solved by statistical simulations
 - Estimation of the probability when tossing a die or dice
 - Ratio of the circumference of a circle
 - Efficiency of estimators
 - Breakdown point
 - Correction factors (d_2 and c_4)
 - Hypothesis testing
 - Development of rt.test R package
 - Development of weibullness R package

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Definition of Statistical Simulation

Definition (wikipedia)

Monte Carlo methods (or Monte Carlo experiments) are a broad class of computational algorithms that rely on **repeated random sampling** to obtain numerical results. Their essential idea is using randomness to solve problems that might be **deterministic in principle**. They are often used in physical and mathematical problems and are most useful when it is difficult or impossible to use other approaches. *Monte Carlo methods are mainly used in three(actually much more?) problem classes*: optimization, numerical integration, and generating draws from a probability distribution.

- ullet Monte Carlo methods \Longrightarrow statistical or stochastic simulation.
- It can solve **stochastic** and **deterministic** problems.
- More applications in statistics: power, distribution, efficiency, bias-correction, etc.

Tips for Simulation

From my teaching experience, many students are confused with:

- sample size *n* and
- the iteration (replication) number 1.
- Sample size n is in general the number of random variable(s).
- The iteration number *I* is the number of repeated experiments.

Problems can be solved by statistical simulations

In this talk, we will solve various problems by statistical simulations.

- Estimation of the probability when tossing a die or dice.
- 2 The ratio of the circumference of a circle, $\pi=3.14...$
- 3 Efficiency of estimators.
- Breakdown point.
- **5** Bias correction factors $(d_2 \text{ and } c_4)$ in Quality Control Chart.
- Hypothesis testing.
- R package (rt.test)
- R package (weibullness)

(1) Estimation of the probability

We are interested in the probability when tossing a single die.

R Code for tossing a fair die

```
set.seed(1)
ITER = 10
x = sample(1:6, size=ITER, replace=TRUE)
table(x) / ITER
table( factor(x, levels=1:6)) / ITER # cosmetic
```

What is the prob. of sum of two outcomes when tossing two dice.

R Code for tossing two dice (sum of two)

```
set.seed(1)
ITER = 10
x = sample(1:6, size=ITER, replace=TRUE)
y = sample(1:6, size=ITER, replace=TRUE)
table(x+y) / ITER
table(factor(x+y, levels=1:12)) / ITER # cosmetic
```

(1) Estimation of the probability

- Homework: 1. Find the probability of the difference of two dice.
 - 2. What if a die is not fair?

(2) Ratio of the circumference of a circle, $\pi = 3.14...$

The idea is very simple — consider a dart game.

The probability that a pin drops in a circle when a pin was thrown at random is given by:

$$\frac{\pi}{4} = \frac{\text{Area of unit circle}}{\text{Area of square}} \approx \frac{\# \text{ of pins in a circle}}{\# \text{ of all the pins}} = \hat{\rho}.$$

Thus, we have $\pi \approx 4 \times \hat{p}$.

♦ NB: Avoid using for() loop in R.

R Code for finding $\pi = 3.14...$

```
set.seed(1)
ITER = 100
x = runif(ITER, min=-1, max=1)
y = runif(ITER, min=-1, max=1)
4 * sum (x^2 + y^2 < 1) / ITER</pre>
```

Also, refer to Talk-1 at seminar.



(2) Ratio of the circumference of a circle, $\pi = 3.14...$

(3) Efficiency of Estimators (mean, median, HL)

The relative efficiency of $\hat{ heta}_2$ given $\hat{ heta}_1$ is defined as

$$RE(\hat{\theta}_2, \hat{\theta}_1) = \frac{Var(\hat{\theta}_1)}{Var(\hat{\theta}_2)} \times 100\%$$
(1)

where $\hat{\theta}_1$ is often a reference or baseline estimator (usually MLE).

Breakdown Points and AREs of the estimators under consideration.

	Location			Scale			
	Mean	Median	HL	SD	IQR	MAD	Shamos
ARE	100%	64%	96%	100%	38%	37%	86%
Breakdown	0%	50%	29%	0%	25%	50%	29%

- Refer to §2.2 of Lehmann Lehmann (1999), Rousseeuw and Croux (1993) and Serfling (2011); Staudte and Sheather (1990).
- HL = $median(X_i + X_j)/2$ for all i < j or $i \le j$. Refer to Talk-2 at •seminar.

(3) Efficiency of Estimators (mean, median, HL)

Here, we will focus on RE or ARE of median and HL with mean as a baseline.

R Code for Relative Efficiency

```
# Load Hodges-Lehmann and Shamos estimators.
source("https://raw.githubusercontent.com/AppliedStat/seminar/master/2018/R/Rsec.R"
TTER = 1000
n = 50
means = medians = HLs = numeric(ITER)
for ( i in 1:ITER ) {
    x = rnorm(n)
    means[i] = mean(x)
    medians[i] = median(x)
    HLs[i] = HL(x)
c( var(means) / var(medians), var(means) / var(HLs) )
```

 $\Diamond NB$: As $n \to \infty$ and $I \to \infty$, RE converges to ARE.

(4) Breakdown point

Definition (Breakdown point)

The finite-sample breakdown point is the maximum proportion of incorrect observations ($\underline{\text{i.e.}}$ arbitrarily large observations) that an estimator can handle without leading to an egregiously incorrect estimate.

R Code for Breakdown point

```
n = 100  # Number of observations
k = 20  # Number of contaminated obs.
x = c(runif(n-k), rep(Inf,k))
c(median(x), HL(x))
k / n
```

- Idea: increase k until an estimator breaks down.
- Try $k = 28, 29, 30, \dots, 49, 50, 51$.

(4) Breakdown point

R Code for Breakdown point (a better code)

```
n = 100  # Number of observations
for ( k in 1: (n/2) ) {  # repeat with a different k
        x = c(runif(n-k), rep(Inf,k))
        print( c(k/n,median(x),HL(x)) )
}
```

- We obtained the finite-sample breakdown point.
- As increase n along with k, we can find the finite-sample breakdown point.
- \Diamond The breakdown point of the median is 1/2 and that of the Hodges-Lehmann is $1-1/\sqrt{2}=0.29289$. Also, refer to Talk-2 at verminar.

(5-1) Bias correction factor (d_2)

The range, $R = X_{(n)} - X_{(1)}$, is not unbiased under the normality assumption. To make it unbiased, we adjust R with the correction factor d_2 so that R/d_2 is unbiased, that is, $E[R/d_2] = \sigma$. Then we have

$$d_2=\frac{1}{\sigma}E[R].$$

Note that we have $X = \sigma Z + \mu$, where Z is from N(0,1). Thus, we have

$$d_2 = E[Z_{(n)} - Z_{(1)}] = 2 \int_0^\infty \left\{ 1 - \left[\Phi(z) \right]^n - \left[1 - \Phi(z) \right]^n \right\} dz,$$

Statistical Simulation

where $\Phi(\cdot)$ is the CDF of N(0,1).

Refer to Section 1 of Talk-5-extra.pdf at seminar.

- To prove the above, it takes almost ten pages.
- d_2 depends on the sample size n.

(5-1) Bias correction factor (d_2)

Idea for estimating E[Y].

The theoretical expectation E[Y] is approximated by

$$\frac{1}{I}\sum_{i=1}^{I}Y_{i}.$$

Since $d_2 = E[Z_{(n)} - Z_{(1)}] = E[Z_{(n)}] - E[Z_{(1)}]$, we have

$$E[Z_{(n)}] \approx \frac{1}{I} \sum_{i=1}^{I} \max_{i} \text{ and } E[Z_{(1)}] \approx \frac{1}{I} \sum_{i=1}^{I} \min_{i},$$

where \max_i and \min_i are the maximum and minimum from a sample of size \boxed{n} at the \boxed{i} th iteration.

(5-1) Bias correction factor (d_2)

R Code for d_2

```
set.seed(1)
n = 10  # sample size
ITER = 1E4  # The larger, the more accurate d2
MAX = MIN = numeric(ITER)
for ( i in 1:ITER ) {
    Z = rnorm(n)
    MAX[i] = max(Z)
    MIN[i] = min(Z)
}
mean(MAX) - mean(MIN)
```

- Better R codes are provided in Section 1 of Talk-5-extra.pdf at seminar.
- For n = 10, we have $d_2 = 3.078$ from the quality control textbook.
- The value through the simulation is given by $d_2 = 3.092639$.

(5-2) Bias correction factor (c_4)

It is well know that the sample variance S^2 is **unbiased** under the normal distribution assumption. That is

$$E[S^2] = \sigma^2,$$

where $S^2 = \sum_{i=1}^n (X_i - \bar{X})^2 / (n-1)$. However, the sample standard deviation S is **not** unbiased so that

$$E[S] \neq \sigma$$
.

Most quality control textbooks use the correction factor, c_4 , so that $E[S/c_4] = \sigma$. The correction factor c_4 is theoretically derived as

$$c_4 = \sqrt{\frac{2}{n-1}} \cdot \frac{\Gamma(n/2)}{\Gamma(n/2-1/2)}.$$

Note that c_4 is an unbiasing factor which is a function of sample size and it was originally used in ASTM E-11 (1976).

Refer to Section 2 of Talk-5-extra.pdf at seminar.

(5-2) Bias correction factor (c_4)

Since $E[S/c_4] = \sigma$, we have $c_4 = \frac{1}{\sigma}E[S] = E[S/\sigma]$. Note that S/σ is a **pivot**. Similar to the case of the range R, we have

$$c_4 = E[S_Z],$$

where S_Z is the sample standard deviation with a sample of size n from N(0,1).

R Code for d_2

(5-3) Comparing R, R/d_2 , S, S/c_4

We have studied R, R/d_2 , S, and S/c_4 .

Then, are R/d_2 and S/c_4 better?

We usually check the bias and variance (or relative efficiency).

Let $\hat{\theta}_i$ be the *i*th estimate from the simulation. Then the empirical bias and variance are given by

Empirical bias:

$$\frac{1}{I}\sum_{i=1}^{I}\hat{\theta}_{i}-\theta.$$

• Empirical variance:

$$\frac{1}{I-1}\sum_{i=1}^{I}(\hat{\theta}_i-\bar{\hat{\theta}})^2.$$

♦ NB: Based on the above variance, we can estimate the relative efficiency.

(5-3) Comparing R, R/d_2 , S, S/c_4

R Code for empirical bias and variance

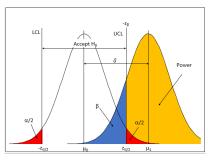
```
# Load Hodges-Lehmann and Shamos estimators.
source("https://raw.githubusercontent.com/AppliedStat/seminar/master/2018/R/Rsec.R"
set.seed(1)
ITER = 1E5
R = Rd2 = SD = SDc4 = numeric(ITER)
for ( i in 1:ITER ) {
    X = rnorm(n)
    R[i] = diff(range(X))
    SD[i] = sd(X)
Rd2 = R / d2(n)
SDc4 = SD / c4(n)
# Bias of estimators
c(mean(R)-1, mean(Rd2)-1, mean(SD)-1, mean(SDc4)-1)
# Var. of estimators
c(var(R), var(Rd2), var(SD), var(SDc4))
```

(6) Hypothesis testing

Consider the statistical hypothesis testing:

$$H_0: \mu = \mu_0$$
 versus $H_1: \mu \neq \mu_0$.

	Decision $H_0 \hspace{1cm} H_1$				
Luth H₀	$egin{array}{c} \mathbf{OK} \ (coverage) \ (1-lpha) \end{array}$	Type-I error (α)			
른 H ₁	Type-II error (β)	$egin{aligned} \mathbf{OK} & ext{(power)} \ (\mathcal{K}(\cdot) = 1 - eta) \end{aligned}$			



 $\Diamond NB$: Power is usually a function of μ or $\delta = \mu_1 - \mu_0$.

(6-1) Hypothesis testing (Example)

Example 8.5-2 from Hogg et al. (2015)

Let X_1, X_2, \ldots, X_{25} be a random sample from $N(\mu, 100)$. We want to test $H_0: \mu = 60$ versus $H_1: \mu > 60$.

When we decided to reject H_0 if $\bar{X} > 62$ (critical/rejection region), find the power function of μ .

Since n=25 and $X_i\sim N(\mu,100)$, we have $\bar{X}\sim N(\mu,100/25)$. Then $Z=(\bar{X}-\mu)/\sqrt{100/25}=(\bar{X}-\mu)/2\sim N(0,1)$. Thus, under $H_1:\mu$, the power function is given by

$$K(\mu) = P[\bar{X} > 62 \mid \mu]$$

$$= P\left[\frac{\bar{X} - \mu}{2} > \frac{62 - \mu}{2}\right] = P\left[Z > \frac{62 - \mu}{2}\right]$$

$$= 1 - \Phi\left[\frac{62 - \mu}{2}\right].$$

(6-1) Hypothesis testing (Example: Power)

Example 8.5-2 from Hogg et al. (2015)

The example state that the power at $\mu = 65$ is K(65) = 0.9332 ...

R Code for Example 8.5-2

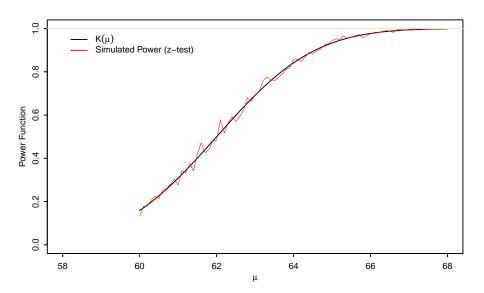
```
# Theoretical power
K = function(mu) \{ 1-pnorm((62-mu)/2) \}
# Empirical power (through simulation)
set.seed(1):
TTER = 10000
n=25; sigma=10; mu=65
count = 0
for ( i in 1:ITER ) {
   X = rnorm(n=n, mean=mu, sd=sigma)
    # count if it is in a critical region.
    if (mean(X) > 62) count = count+1
c( count / ITER, K(65) )
```

(6-1) Hypothesis testing (Power function)

R Code for Figure 8.5-2: Power function $K(\mu)$

```
# Empirical power (through simulation)
set.seed(1)
TTER = 1000
n=25; sigma=10; MU=seq(60, 68, length=81)
power = numeric(length(MU))
for ( j in 1:length(MU) ) {
   mu = MU[j]
    for ( i in 1:ITER ) {
        X = rnorm(n=n, mean=mu, sd=sigma)
        if (mean(X) >= 62) power[j] = power[j] + 1/ITER
 Compare the empirical power with the theoretical power
plot(MU, K(MU), xlim=c(58,68), ylim=c(0,1), type="l")
lines(MU, power, col="red")
```

(6-1) Hypothesis testing



(6-2) Testing $H_0: \mu = \mu_0$ vs. $H_0: \mu \neq \mu_0$

• σ is known (z-test): reject H_0 if

$$\begin{aligned} |z| &= \frac{|\bar{x} - \mu_0|}{\sigma/\sqrt{n}} > z_{\alpha/2} \\ \mathcal{K}_z(\mu) &= 1 - \Phi\left(z_{\alpha/2} + \frac{\mu - \mu_0}{\sigma/\sqrt{n}}\right) + \Phi\left(-z_{\alpha/2} + \frac{\mu - \mu_0}{\sigma/\sqrt{n}}\right) \end{aligned}$$

• σ is unknown (t-test): reject H_0 if

$$egin{aligned} |t| &= rac{|ar{x} - \mu_0|}{S/\sqrt{n}} > t_{lpha/2}(n-1) \ K_t(\mu) &= 1 - \Phi_{
u,\delta}(t_{lpha/2}) + \Phi_{
u,\delta}(-t_{lpha/2}), \end{aligned}$$

where $\Phi_{\nu,\delta}(\cdot)$ is the CDF of the non-central t-distribution with $\nu=n-1$ degrees of freedom and non-centrality $\delta=(\mu-\mu_0)/(\sigma/\sqrt{n})$.

♦ Refer to Section 3 of Talk-5-extra.pdf at pages!

$\overline{\text{(6-2)}}$ Hypothesis testing (Power function when σ is known)

R Code for empirical power of z-test (σ is known)

```
Kz = function(mu, alpha, mu0, sigma, n) {
    z.cut = qnorm(1-alpha/2)
    tmp = (mu-mu0)/(sigma/sqrt(n))
   pnorm(z.cut + tmp, lower.tail=FALSE) + pnorm(-z.cut + tmp)
# Empirical Power
set.seed(1); ITER = 1E4
mu=1.5; mu0=0.5; alpha=0.05; sigma=1; n=5
power = 0
zcut = qnorm(1-alpha/2)
for ( i in 1:ITER ) {
 X = rnorm(n, mean=mu, sd=1)
  if(abs(mean(X)-mu0)/(sigma/sqrt(n)) > zcut) power=power+1/ITER
}
# Compare
c(Kz(mu, alpha, mu0, sigma, n), power)
```

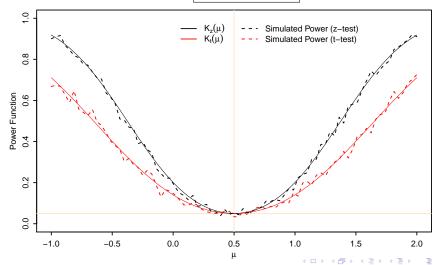
(6-3) Hypothesis testing (Power when σ is unknown)

R Code for empirical power of t-test (σ is unknown)

```
Kt = function(mu, alpha, mu0, sigma, n) {
  t.cut = qt(1-alpha/2,df=n-1)
  ncp = (mu-mu0)/(sigma/sqrt(n))
  pt(t.cut,df=n-1,ncp=ncp,lower.tail=F)+pt(-t.cut,df=n-1,ncp=ncp)
}
# Empirical Power
set.seed(1); ITER = 1E4
mu=1.5; mu0=0.5; alpha=0.05; sigma=1; n=5
power = 0
tcut = qt(1-alpha/2, df=n-1) # tcut is used instead of zcut
for ( i in 1:ITER ) {
 X = rnorm(n, mean=mu, sd=1)
  # sd(X) is used instead of known sigma
  if(abs(mean(X)-mu0)/(sd(X)/sqrt(n)) > tcut) power=power+1/ITER
# Compare
c(Kt(mu, alpha, mu0, sigma, n), power)
```

(6-3) Hypothesis testing: Power

Testing $H_0: \mu=1/2$ versus $H_1: \mu\neq 1/2$ with $\alpha=0.05$, n=5, and $\sigma=1$. Refer to Section 3.3 of Talk-5-extra.pdf at Pseminar.



(7-1) Warming-up before rt.test R package

t-test statistic

$$T = \frac{\bar{X} - \mu}{S_X / \sqrt{n}},\tag{2}$$

where $\bar{X} = \sum X_i/n$, $S_X^2 = \sum (X_i - \bar{X})^2/(n-1)$ and X_i are from $N(\mu, \sigma^2)$. Substituting $X_i = \sigma Z_i + \mu$ into (2), we have

$$T = \frac{Z - \mu}{S_Z / \sqrt{n}},$$

Note that T is a **pivot**.

- Assume that we know only the normal distribution.
- How to know the distribution of T above.



(7-1) Warming-up before rt.test R package

R Code for the critical value of the two-side *t*-test when $\alpha = 5\%$

```
set.seed(1)
ITER = 1.0E4; n=6;
Tstat = numeric(ITER)
for ( i in 1:ITER ) {
    7 = rnorm(n)
   Tstat[i] = mean(Z) / (sd(Z)/sqrt(n))
}
# Critical values
quantile(Tstat, prob=0.975)
qt(0.975, df=n-1)
qnorm(0.975) # 1.96
# Plot
hist(Tstat,breaks=100,probability=T,xlim=c(-5,5),ylim=c(0,0.4))
lines( density(Tstat))
curve( dnorm(x), xlim=c(-5,5), add=T, col="red")
```

(7-2) rt.test R package

Recall a basic idea

$$T = \frac{\bar{X} - \mu}{S / \sqrt{n}} \tag{3}$$

- $|\bar{X}|$ is replaced by median or Hodges and Lehmann (1963).
- S is replaced by MAD or Shamos (1976).
- Is it enough? No.
- Then, is it distributed as N(0,1) or t-distribution? Neither. T_A or $T_B \stackrel{\bullet}{\sim} N(0,1)$ (Refer to KIIE at Seoul, November 2018). Thus, T_A or T_B works for a large sample. What if a sample is small?
- ♦ NB: Refer to Talk-2 at •seminar and rt.test R package at •rt.test.

(7-2) rt.test R package

Recall T_A and T_B

Refer to Park and Wang (2018a) at ArXiv.

$$T_{A} = \sqrt{\frac{2n}{\pi}} \Phi^{-1} \left(\frac{3}{4}\right) \cdot \frac{\underset{1 \le i \le n}{\operatorname{median}} X_{i} - \mu}{\underset{1 \le i \le n}{\operatorname{median}} \left|X_{i} - \underset{1 \le i \le n}{\operatorname{median}} X_{i}\right|} \xrightarrow{d} N(0, 1), \tag{4}$$

where $\Phi^{-1}(\cdot)$ is the inverse of the standard normal cumulative distribution function and $\stackrel{d}{\longrightarrow}$ denotes convergence in distribution.

$$T_B = \sqrt{\frac{6n}{\pi}} \Phi^{-1} \left(\frac{3}{4}\right) \frac{ \underset{i \le j}{\operatorname{median}} \left(\frac{X_i + X_j}{2}\right) - \mu}{ \underset{i \le j}{\operatorname{median}} \left(|X_i - X_j|\right)} \stackrel{d}{\longrightarrow} N(0, 1).$$
 (5)

 \Diamond NB: T_A and T_B are **pivotal**. See Park (2018a) and Jeong et al. (2018).

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(7-2) rt.test R package

R Code for the critical value of rt.test R package

```
set.seed(1)
ITER = 1.0E4; n=6;
TA = numeric(ITER)
for ( i in 1:ITER ) {
    7 = rnorm(n)
   TA[i] = sqrt(2*n/pi)*qnorm(3/4)*median(Z)/mad(Z,constant=1)
}
# Install rt.test package
install.packages("rt.test")
library("rt.test")
# Critical values
quantile(TA, prob=0.975)
q.robustified.t(0.975, n=n) # This Package used ITER = 1.0E8
qnorm(0.975) # 1.96 (compare it with the above)
```

Recall: Weibull distribution (reparametrized form)

$$F(x) = 1 - \exp(-\lambda x^{\alpha})$$
 and $f(x) = \lambda \alpha x^{\alpha-1} \exp(-\lambda x^{\alpha})$,

It is immediate from the Weibull CDF F(x) = p that

$$\log(1-p) = -\lambda x_p^{\alpha}.$$

It follows that

$$\log\big\{-\log(1-p)\big\} = \log\lambda + \alpha\log x_p.$$

This implies that the plot of

$$\log \left\{ -\log(1-p) \right\}$$
 versus $\log x_p$

draws a straight line with the slope α and the intercept $\log \lambda$.

 \Diamond NB: Refer to Park (2017) and Talk-3 at seminar and weibullness R package at seminar.

Recall: How to determine whether the data are from Weibull or not

 H_0 : Weibull versus H_1 : non-Weibull.

- Recall: $\log \{ -\log(1-p) \} = \log \lambda + \alpha \log x_p$.
- Thus $\log \left\{ -\log(1-\hat{p}_i) \right\}$ versus $\log x_{(i)}$ draws a straight line, where $\hat{p}_i = (i-0.375)/(n+0.25)$. Thus, the linearity measure (sample correlation) can be used for Weibullness test.
- Idea: Large *r* implies Weibullness.

$$H_0: r \ge r_0$$
 versus $H_1: r < r_0$

Then, how small is small enough for r to reject H_0 ?

- To this end, we should know the distribution of *r* and then find the critical value.
- \Diamond NB: r is a **pivot**. Thus, for Weibull with any parameter values, the results are the same. \Longrightarrow Use exponential distribution with rate one.

Algorithm

- Step-1: Generate Weibull random observations of size n from any Weibull. Note Weibull(1,1) is an exponential distribution.
- Step-2: Sort the data. Denote $x_{(i)}$.
- Step-3: Calculate $\log \{ -\log(1-\hat{p}_i) \}$, where $\hat{p}_i = (i-0.375)/(n+0.25)$ or $\hat{p}_i = (i-0.5)/n$.
- Step-4: Calculate the sample correlation between $\log \left\{ -\log(1-\hat{p}_i) \right\}$ and $\log x_{(i)}$.
- Step-5: Repeat the above (say, up to I iteration numbers).
- Step-6: Find the empirical quantiles for critical values (say, 5%, 10%, etc.)
- ♦ NB: Compare the sample correlation with the empirical quantile (critical value) in order to make a decision.

R Code for the critical value of weibullness R package

```
set.seed(1)
ITER = 1.0E4; n=23;
cors = numeric(ITER)
for ( i in 1:ITER ) {
  x = sort(rexp(n)) # Step 1-2
  p = ppoints(n) # Step 3
   cors[i] = cor(log(-log(1-p)), log(x))
                                          # Step 4
} # Repeat (i=1,2,...,ITER)
                                           # Step 5
alphas = c(0.01, 0.02, 0.025, 0.5, 0.1, 0.2)
quantile(cors, prob=alphas)
                                           # Step 6
# Install weibullness package
install.packages("weibullness")
library("weibullness")
wp.test.critical(alphas,n) # This package used ITER=1E8
```

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