

# Sequential Implementation of Monte Carlo Tests with Uniformly Bounded Resampling Risk

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# Introduction

- ▶ Test statistic  $T$ , reject for large values.
- ▶ Observation:  $t$ .
- ▶  $p$ -value:

$$p = P(T \geq t)$$

Often not available in closed form.

- ▶ Monte Carlo Test:

$$\hat{p}_{\text{naive}} = \frac{1}{n} \sum_{i=1}^n \mathbb{I}(T_i \geq t),$$

where  $T, T_1, \dots, T_n$  i.i.d.

- ▶ Examples:
  - ▶ Bootstrap,
  - ▶ Permutation tests.
- ▶ Goal: Estimate  $p$  using few  $X_i$

Mainly interested in deciding if  $p \leq \alpha$  for some  $\alpha$ .

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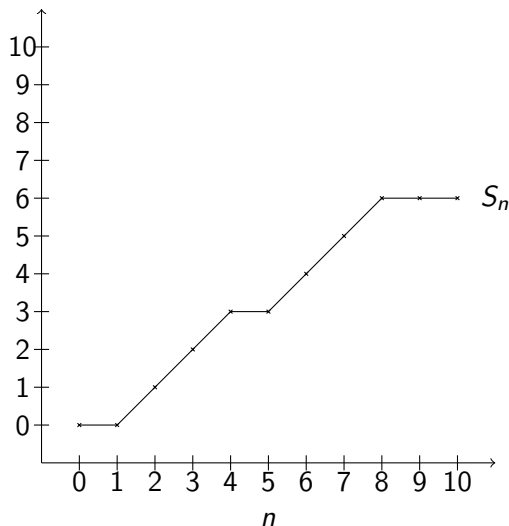
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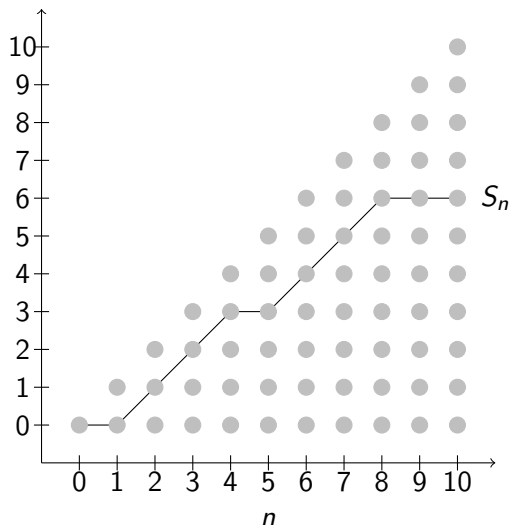
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# Sequential approaches based on $S_n = \sum_{i=1}^n X_i$



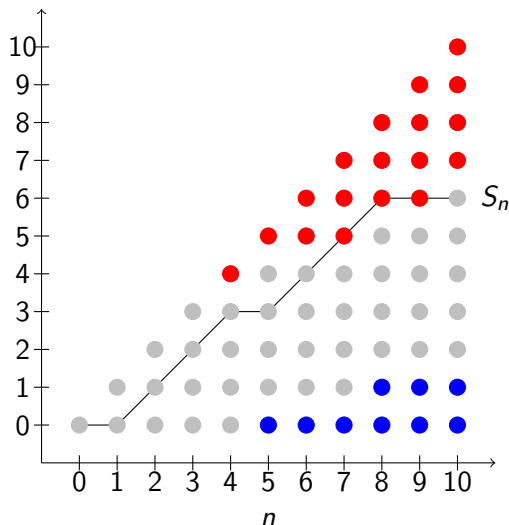
- ▶ Stop once  $S_n \geq U_n$  or  $S_n \leq L_n$
- ▶  $\tau$ : hitting time
- ▶ Compute  $\hat{p}$  based on  $S_\tau$  and  $\tau$ .
- ▶ Hit  $B_U$ : decide  $p > \alpha$ ,
- ▶ Hit  $B_L$ : decide  $p \leq \alpha$ ,

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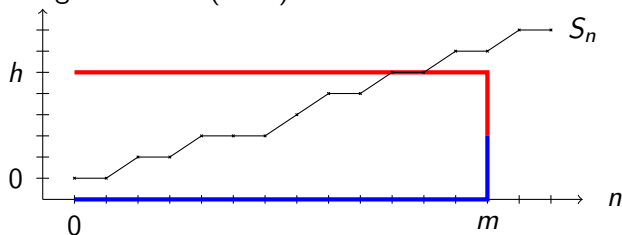


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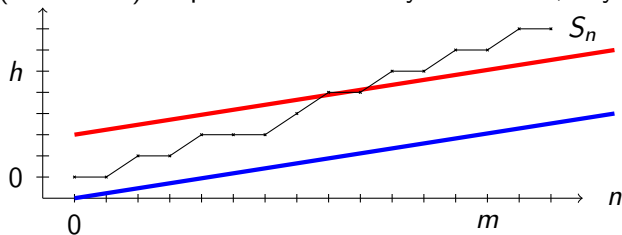


# Previous Approaches

- ▶ Besag & Clifford (1991):



- ▶ (Truncated) Sequential Probability Ratio Test, Fay et al. (2007)



- ▶ R-package `MChtest`.

# What do we really want?

Is  $p \leq \alpha$ ?

Two individuals using the same statistical method on the same data should arrive at the same conclusion.

*First law of applied statistics, Gleser (1996)*

Consider the **resampling risk**

$$RR_p(\hat{p}) \equiv \begin{cases} P_p(\hat{p} > \alpha) & \text{if } p \leq \alpha, \\ P_p(\hat{p} \leq \alpha) & \text{if } p > \alpha. \end{cases}$$

Want:

$$\sup_{p \in [0,1]} RR_p(\hat{p}) \leq \epsilon$$

for some (small)  $\epsilon > 0$ .

For Besag & Clifford (1991), SPRT:  $\sup_p RR_p \geq 0.5$

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# Recursive Definition of the Boundaries

Want:

$$\sup_p \text{RR}_p(\hat{p}) \leq \epsilon$$

Suffices to ensure

$$P_\alpha(\text{hit } B_U) \leq \epsilon$$

$$P_\alpha(\text{hit } B_L) \leq \epsilon$$

Recursive definition:

Choose  $\epsilon_n$  and  $\alpha_n$  such that  $\epsilon_n \nearrow \epsilon$  and  $\alpha_n \nearrow \alpha$

- ▶  $\tau_n$  as the minimal value such that

$$P_{\alpha_n}(\text{hit } B_U \text{ until } n) \leq \epsilon_n$$

- ▶ and  $\tau'_n$  as the maximal value such that

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where  $\epsilon_n \geq 0$  with  $\epsilon_n \nearrow \epsilon$  (**spending sequence**).



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Given  $U_1, \dots, U_{n-1}$  and  $L_1, \dots, L_{n-1}$ , define

- ▶  $U_n$  as the minimal value such that

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## Recursive Definition - Example

- ▶  $\alpha = 0.2$ ,  $\epsilon_n = 0.4 \frac{n}{5+n}$ .
- ▶  $U_n$  = the minimal value such that

$$P_\alpha(\text{hit } B_U \text{ until } n) \leq \epsilon_n$$

- ▶  $L_n$  = maximal value such that

$$P_\alpha(\text{hit } B_L \text{ until } n) \leq \epsilon_n$$

|                                  | $n =$ |
|----------------------------------|-------|
| $P_\alpha(S_n = k, \tau \geq n)$ | 0     |
| $k = 3$                          |       |
| $k = 2$                          |       |
| $k = 1$                          |       |
| $k = 0$                          | 1     |
| $\epsilon_n$                     | 0     |
| $U_n$                            | 1     |
| $L_n$                            | -1    |

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| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |
|----------------------------------|-------|-----|
|                                  | 0     | 1   |
| $k = 3$                          |       |     |
| $k = 2$                          |       |     |
| $k = 1$                          |       | .2  |
| $k = 0$                          | 1     | .8  |
| $\epsilon_n$                     | 0     | .07 |
| $U_n$                            | 1     | 2   |
| $L_n$                            | -1    | -1  |

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|                                  | $n =$ |     |     |
|----------------------------------|-------|-----|-----|
| $P_\alpha(S_n = k, \tau \geq n)$ | 0     | 1   | 2   |
| $k = 3$                          |       |     |     |
| $k = 2$                          |       |     | .04 |
| $k = 1$                          |       | .2  | .32 |
| $k = 0$                          | 1     | .8  | .64 |
| $\epsilon_n$                     | 0     | .07 | .11 |
| $U_n$                            | 1     | 2   | 2   |
| $L_n$                            | -1    | -1  | -1  |

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|                                  | $n =$ |     |     |     |
|----------------------------------|-------|-----|-----|-----|
| $P_\alpha(S_n = k, \tau \geq n)$ | 0     | 1   | 2   | 3   |
| $k = 3$                          |       |     |     |     |
| $k = 2$                          |       |     | .04 | .06 |
| $k = 1$                          |       | .2  | .32 | .38 |
| $k = 0$                          | 1     | .8  | .64 | .51 |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 |
| $U_n$                            | 1     | 2   | 2   | 2   |
| $L_n$                            | -1    | -1  | -1  | -1  |

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| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |     |     |     |
|----------------------------------|-------|-----|-----|-----|-----|
|                                  | 0     | 1   | 2   | 3   | 4   |
| $k = 3$                          |       |     |     |     |     |
| $k = 2$                          |       |     | .04 | .06 | .08 |
| $k = 1$                          |       | .2  | .32 | .38 | .41 |
| $k = 0$                          | 1     | .8  | .64 | .51 | .41 |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 | .18 |
| $U_n$                            | 1     | 2   | 2   | 2   | 3   |
| $L_n$                            | -1    | -1  | -1  | -1  | -1  |



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| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |     |     |     |     |
|----------------------------------|-------|-----|-----|-----|-----|-----|
|                                  | 0     | 1   | 2   | 3   | 4   | 5   |
| $k = 3$                          |       |     |     |     |     | .02 |
| $k = 2$                          |       |     | .04 | .06 | .08 | .14 |
| $k = 1$                          |       | .2  | .32 | .38 | .41 | .41 |
| $k = 0$                          | 1     | .8  | .64 | .51 | .41 | .33 |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 | .18 | .20 |
| $U_n$                            | 1     | 2   | 2   | 2   | 3   | 3   |
| $L_n$                            | -1    | -1  | -1  | -1  | -1  | -1  |

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| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |     |     |     |     |     |
|----------------------------------|-------|-----|-----|-----|-----|-----|-----|
|                                  | 0     | 1   | 2   | 3   | 4   | 5   | 6   |
| $k=3$                            |       |     |     |     |     | .02 | .03 |
| $k=2$                            |       |     | .04 | .06 | .08 | .14 | .20 |
| $k=1$                            |       | .2  | .32 | .38 | .41 | .41 | .39 |
| $k=0$                            | 1     | .8  | .64 | .51 | .41 | .33 | .26 |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 | .18 | .20 | .22 |
| $U_n$                            | 1     | 2   | 2   | 2   | 3   | 3   | 3   |
| $L_n$                            | -1    | -1  | -1  | -1  | -1  | -1  | -1  |

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| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |     |     |     |     |     |     |
|----------------------------------|-------|-----|-----|-----|-----|-----|-----|-----|
|                                  | 0     | 1   | 2   | 3   | 4   | 5   | 6   | 7   |
| $k=3$                            |       |     |     |     |     | .02 | .03 | .04 |
| $k=2$                            |       |     | .04 | .06 | .08 | .14 | .20 | .24 |
| $k=1$                            |       | .2  | .32 | .38 | .41 | .41 | .39 | .37 |
| $k=0$                            | 1     | .8  | .64 | .51 | .41 | .33 | .26 | .21 |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 | .18 | .20 | .22 | .23 |
| $U_n$                            | 1     | 2   | 2   | 2   | 3   | 3   | 3   | 3   |
| $L_n$                            | -1    | -1  | -1  | -1  | -1  | -1  | -1  | 0   |

## Recursive Definition - Example

- ▶  $\alpha = 0.2$ ,  $\epsilon_n = 0.4 \frac{n}{5+n}$ .
- ▶  $U_n$  = the minimal value such that

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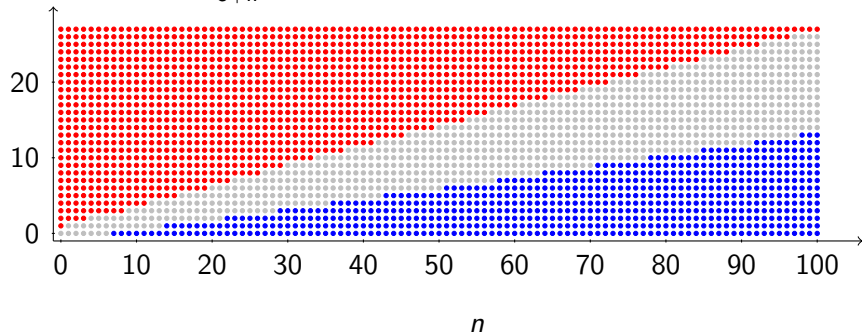
- ▶  $L_n$  = maximal value such that

$$P_\alpha(\text{hit } B_L \text{ until } n) \leq \epsilon_n$$

| $P_\alpha(S_n = k, \tau \geq n)$ | $n =$ |     |     |     |     |     |     |     |     |  |
|----------------------------------|-------|-----|-----|-----|-----|-----|-----|-----|-----|--|
|                                  | 0     | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   |  |
| $k=3$                            |       |     |     |     |     | .02 | .03 | .04 | .05 |  |
| $k=2$                            |       |     | .04 | .06 | .08 | .14 | .20 | .24 | .26 |  |
| $k=1$                            |       | .2  | .32 | .38 | .41 | .41 | .39 | .37 | .29 |  |
| $k=0$                            | 1     | .8  | .64 | .51 | .41 | .33 | .26 | .21 |     |  |
| $\epsilon_n$                     | 0     | .07 | .11 | .15 | .18 | .20 | .22 | .23 | .25 |  |
| $U_n$                            | 1     | 2   | 2   | 2   | 3   | 3   | 3   | 3   | 3   |  |
| $L_n$                            | -1    | -1  | -1  | -1  | -1  | -1  | -1  | 0   | 0   |  |

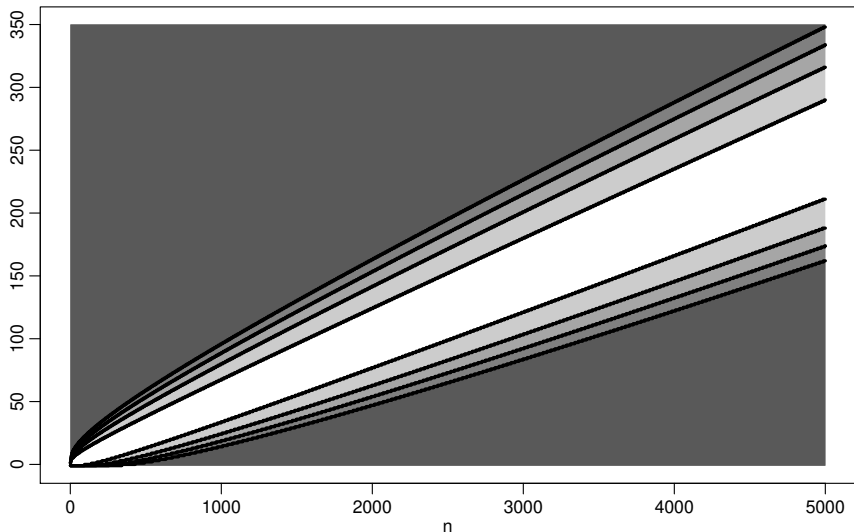
# Sequential Decision Procedure - Example

$$\alpha = 0.2, \epsilon_n = 0.4 \frac{n}{5+n}.$$



# Influence of $\epsilon$ on the stopping rule

$$\epsilon = 0.1, 0.001, 10^{-5}, 10^{-7}; \epsilon_n = \epsilon \frac{n}{1000+n}$$



# Sequential Estimation based on the MLE

$$\hat{p} = \begin{cases} \frac{S_\tau}{\tau}, & \tau < \infty \\ \alpha, & \tau = \infty, \end{cases}$$

- ▶ One can show:
  - ▶ hitting the upper boundary implies  $\hat{p} > \alpha$ ,
  - ▶ hitting the lower boundary implies  $\hat{p} < \alpha$ .

Hence,

$$\sup_p \text{RR}_p(\hat{p}) \leq \epsilon$$

- ▶ Furthermore,  $\exists$  random interval  $I_n$  s.t.
  - ▶  $I_n$  only depends on  $X_1, \dots, X_n$ ,
  - ▶  $\hat{p} \in I_n$ .

## Example - Two-way sparse contingency table

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 1 | 1 | 0 | 1 |
| 2 | 0 | 0 | 2 | 3 | 0 | 0 |
| 0 | 1 | 1 | 1 | 2 | 7 | 3 |
| 1 | 1 | 2 | 0 | 0 | 0 | 1 |
| 0 | 1 | 1 | 1 | 1 | 0 | 0 |

- ▶  $H_0$ : variables are independent.
- ▶ Reject for large values of the likelihood ratio test statistic  $T$
- ▶  $T \xrightarrow{d} \chi^2_{(7-1)(5-1)}$  under  $H_0$ . Based on this:  $p = 0.031$ .
- ▶ Matrix sparse - approximation poor?
- ▶ Use parametric bootstrap based on row and column sums.
- ▶ Naive test statistic  $\hat{p}_{naive}$  with  $n = 1,000$  replicates:  
 $p = 0.041 < 0.05$ .  
Probability of reporting  $p > 0.05$ : roughly 0.08.



## Example - Two-way sparse contingency table

|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 1 | 2 | 2 | 1 | 1 | 0 | 1 |
| 2 | 0 | 0 | 2 | 3 | 0 | 0 |
| 0 | 1 | 1 | 1 | 2 | 7 | 3 |
| 1 | 1 | 2 | 0 | 0 | 0 | 1 |
| 0 | 1 | 1 | 1 | 1 | 0 | 0 |

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## Example - Bootstrap and Sequential Algorithm

```
> dat <- matrix(c(1,2,2,1,1,0,1, 2,0,0,2,3,0,0, 0,1,1,1,2,7,3, 1,1,2,0,0,0,1,
+               0,1,1,1,1,0,0), nrow=5,ncol=7,byrow=TRUE)
> loglikrat <- function(data){
+   cs <- colSums(data);rs <- rowSums(data); mu <- outer(rs,cs)/sum(rs)
+   2*sum(iffelse(data<=0.5, 0,data*log(data/mu)))
+ }
> resample <- function(data){
+   cs <- colSums(data);rs <- rowSums(data); n <- sum(rs)
+   mu <- outer(rs,cs)/n/n
+   matrix(rmultinom(1,n,c(mu)),nrow=dim(data)[1],ncol=dim(data)[2])
+ }
> t <- loglikrat(dat);
> library(simctest)
> res <- simctest(function(){loglikrat(resample(dat))}>=t},maxsteps=1000)
> res
No decision reached.
Final estimate will be in [ 0.02859135 , 0.07965451 ]
Current estimate of the p.value: 0.041
Number of samples: 1000
> cont(res, steps=10000)
p.value: 0.04035456
Number of samples: 8574
```

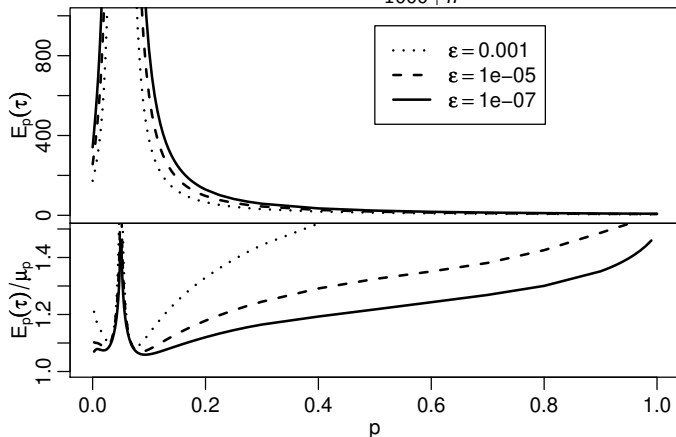
## Further Uses of the Algorithm

- ▶ Simulation study to evaluate whether a test is liberal/conservative.
- ▶ Determining the sample size to achieve a certain power.
- ▶ Iterated Use:
  - ▶ Determining the power of a bootstrap test.
  - ▶ Simulation study to evaluate whether a bootstrap test is liberal/conservative.
  - ▶ Double bootstrap test.

# Expected Hitting Time

Result:  $E_p(\tau) < \infty \forall p \neq \alpha$

Example with  $\alpha = 0.05$ ,  $\epsilon_n = \epsilon \frac{n}{1000+n}$ :



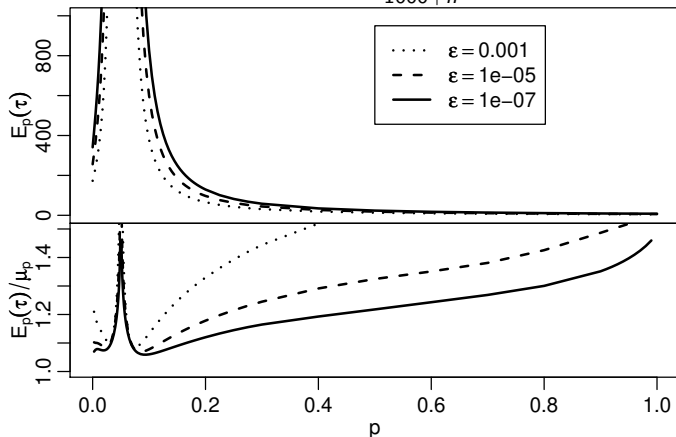
$\mu_p$  = theoretical lower bound on  $E_p(\tau)$ .

- ▶ Note:  $\int_0^1 \mu_p dp = \infty$ ;
- ▶ for iterated use: Need to limit the number of steps.

## Expected Hitting Time

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# Summary

- ▶ Sequential implementation of Monte Carlo Tests and computation of  $p$ -values.
- ▶ Useful when implementing tests in packages.
- ▶ After a finite number of steps:
  - ▶  $\hat{p}$  or
  - ▶ interval  $[\hat{p}_n^L, \hat{p}_n^U]$  in which  $\hat{p}$  will lie.
- ▶ Guarantee (up to a very small error probability):  
 $\hat{p}$  is on the “correct side” of  $\alpha$ .
- ▶ R-package [simctest](#) available on CRAN.  
(efficient implementation with C-code)
- ▶ For details see Gandy (2009).

# References

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