Best practices for using simulation studies to evaluate statistical methods

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Overview

Today, we cover:

- Simulation studies
  - Design
  - Implementation
  - Presentation
- Lab

Announcements

- HW2 posted and due 1/28 at 10:00AM

Motivation

- In statistics, simulations are typically used to establish **properties** of statistical methods, particularly when it is difficult or impossible to derive **exact analytic expressions**:
  - Is my estimator biased in finite samples?
  - Does my confidence interval achieve nominal coverage?
  - How powerful is my test under different alternatives to the null hypothesis?
  - How does my method compare to a competing method?
- Exact or approximate analytic results may require assumptions
  - e.g. normality
  - Simulations can be used to study behavior when these assumptions are violated

Monte Carlo Simulation

- The questions on the previous slides can be answered using **Monte Carlo simulation**
- A Monte Carlo simulation is a computer experiment involving (pseudo-)random sampling
- Simulation is used for:
  - Simulation studies (focus of this lecture)
  - Multiple imputation methods
  - Markov Chain Monte Carlo methods (focus of later lectures)

Monte Carlo History

- New supercomputer (ENIAC) inspired former Manhattan Project scientists Stan Ulam and John von Neumann to try a statistical approach to solving an intractable system of equations related to creation of an atomic bomb

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THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM
Los Alamos Laboratory

Monte Carlo History

- Ulam was playing solitaire and wondered: what are the chances that a hand laid out with 52 cards will come out successfully?
    - $\sim 8 \times 10^{67}$ ways to sort a deck of cards
        - Intractable analytically
- What if instead he could simply lay out the cards one hundred times and count the number of successful plays?

Simulation studies in biostatistics

Many uses!

- Check algebra (and code) to provide reassurance no error has been made when a new statistical method has been derived analytically
- Assess relevance of large-sample theory in finite samples
- For absolute evaluation of a new method
  - Does it work well in the scenarios for which it was designed?
- For comparative evaluation of two or more methods

Simulation Study Design

- Simulation studies are **empirical experiments**
- As statisticians, we should apply principles of **experimental design** when conducting simulation studies
- Burton, Altman, Royston, and Holder (2006): Before writing code, develop a **protocol** that provides details about how the study will be performed, analysed, and reported

Simulation Study Design

- Morris, White, and Crowther (2019) advocate for **ADEMP**:
  - Aims
  - Data-generating Mechanisms
  - Estimands
  - Methods
  - Performance Measures

ADEMP Structure

Aims	3.1
· Identify *specific* aims of simulation study.	
Data-generating mechanisms	3.2
· In relation to the aims, decide whether to use resampling or simulation from some parametric model.	
· For simulation from a parametric model, decide how simple or complex the model should be and whether it should be based on real data.	
· Determine what factors to vary and the levels of factors to use.	
· Decide whether factors should be varied fully factorially, partly factorially or one-at-a-time.	
Estimand/target of analysis	3.3
· Define estimands and/or other targets of the simulation study.	
Methods	3.4
· Identify methods to be evaluated and consider whether they are appropriate for estimand/target identified. For method comparison studies, make a careful review of the literature to ensure inclusion of relevant methods.	
Performance measures	3.5, 5.2
· List all performance measures to be estimated, justifying their relevance to estimands or other targets.	
· For less-used performance measures, give explicit formulae for the avoidance of ambiguity.	5.2
· Choose a value of n_{sim} that achieves acceptable Monte Carlo SE for key performance measures.	5.2, 5.3

Planning Stage (notation)

θ	An estimand (conceptually); also true value of the estimand
n_{obs}	Sample size of a simulated dataset
n_{sim}	Number of repetitions used; the simulation sample size
$i = 1, \dots, n_{\text{sim}}$	Indexes the repetitions of the simulation
$\hat{\theta}$	the estimator of θ
$\hat{\theta}_i$	the estimate of θ from the ith repetition
$\bar{\theta}$	the mean of $\hat{\theta}_i$ across repetitions
$\text{Var}(\hat{\theta})$	the true variance of $\hat{\theta}$, which can be estimated with large n_{sim}
$\widehat{\text{Var}}(\hat{\theta}_i)$	an estimate of $\text{Var}(\hat{\theta})$ from the ith repetition
α	the nominal significance level
p_i	the p-value returned by the ith repetition

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- An estimand is the precise quantity or parameter of interest that a study aims to estimate to address its research question.

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Example: treatment effect in a clinical trial

Simple exam: linear regression

$$Y_i = \beta_0 + \beta_{treatment} X_{i1} + \mathbf{Z_i}^T \gamma + \epsilon_i$$

- Y_i: continuous outcome
- X_{i1}: treatment group indicator; $X_{i1} = 1$ for treated
- $\mathbf{Z_i}$: vector of potental confounders
- $\beta_{treatment}$: average treatment effect, adjusting for $\mathbf{Z_i}$
- γ: vector of regression coefficient values for confounders
- ϵ_i: iid error, $\sim N(0, \sigma^2)$

Planning Stage: Aims

Desirable (asymptotic) properties of an estimator $\hat{\theta}$ from a frequentist perspective:

1. $\hat{\theta}$ should be consistent: as $n \to \infty$, $\hat{\theta} \to \theta$
   - Also desirable that $\hat{\theta}$ is unbiased: $E(\hat{\theta}) = \theta$
2. The sample estimate $\widehat{Var(\hat{\theta})}$ consistent estimate of true sampling variance of $\hat{\theta}$, $Var(\hat{\theta})$
3. Confidence intervals should have **good coverage**: at least $100(1-\alpha)\%$ of intervals contain θ
4. $\hat{\theta}$ should be efficient: $Var(\hat{\theta})$ should be as small as possible

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4. $\hat{\theta}$ should be efficient: $Var(\hat{\theta})$ should be as small as possible

Planning Stage: Aims

Proof-of-concept vs. stretching simulation studies

- Proof-of-concept: aim to show that a method is viable in some settings
- Stretch/break objective:: identify settings where the method may fail

Examples of each in the linear regression setting?

Data-generating mechanisms

Refers to how random numbers are used to generate a simulated dataset.

1. Parametric draws from a known model
    - true data generating model is known
    - more flexible but may be overly simplistic for real data
2. Repeated resampling with replacement from a specific dataset
    - true data generating model is unknown
    - less flexible but relevant for at least the study at hand

Data-generating mechanisms

If using a parametric model, need to fully specify your generative model:

- Functional form(s)
- True values of the parameters
- Error distributions and their parameters

Without every detail of the data generation process, others will not be able to reproduce your simulation results!

Data-generating mechanisms

Suppose you want to calculate coverage for $\hat{\beta}_{treatment}$ under several conditions:

- Sample sizes $n \in \{50, 100, 200\}$
- Error variances $\sigma^2 \in \{1, 3\}$
- True treatment effects $\beta_{treatment} \in \{0, 0.5, 2\}$
- **Full factorial design**: evaluate all combinations of these conditions/factors
  - $3 \times 2 \times 3 = 18$ simulation scenarios
  - This is the preferred approach, but can be computationally demanding

Estimands and other targets

- Most simulation studies evaluate or compare methods for estimating one or more population quantities, which we term **estimands** and denote by θ
- Choice of estimand(s) depends on the aims of your study!
  - If you are interested in how well treatment works: $\beta_{treatment}$
  - If interested in the patient outcome value for a given set of characteristics: $E(Y_i|X_i, \beta)$
- Not all simulation studies involve an estimand. These other quantities we might want to focus on are referred to as **targets** of a simulation study

Estimands and other targets

Statistical Task	Target	Examples of Performance Measures
Analysis		
Estimation	Estimand	Bias, empirical SE, mean-squared error, coverage
Testing	Null hypothesis	Type I error rate, power
Model selection	Model	Correct model rate, sensitivity or specificity for covariate selection
Prediction	Prediction/s	Measures of predictive accuracy, calibration, discrimination
Design		
Design a study	Selected design	Sample size, expected sample size, power/precision

Planning: Methods

What method is being evaluated? Is it being compared to other methods?

- When comparing across multiple methods, it is important to consider:
    - Are all relevant methods in the literature being included in your study?
        - If not, what is your justification?
    - Do competing methods have open source implementations?
        - Will you need to contact author(s) for code?
    - What are the assumptions of each method?
        - Will your simulation design favor one method over another?

Planning: Performance measures

A **performance measure** is a numerical quantity used to assess the performance of a method. Examples of common measures:

- bias: $E[\widehat{\theta}] - \theta$
    - used for estimands
- coverage: $Pr(\widehat{\theta}_{low} \leq \theta \leq \widehat{\theta}_{high})$
    - used for estimands
- power and type 1 error
    - used in evaluating a method that targets a hypothesis test

Implementing the simulation study

CODING AND EXECUTION	4
· Separate scripts used to analyze simulated datasets from scripts to analyze estimates datasets.	
· Start small and build up code, including plenty of checks.	
· Set the random number seed once per simulation repetition.	
· Store the random number states at the start of each repetition.	
· If running chunks of the simulation in parallel, use separate streams of random numbers.[17]	
ANALYSIS	5
· Conduct exploratory analysis of results, particularly graphical exploration.	
· Compute estimates of performance and Monte Carlo SEs for these estimates.	5.2
REPORTING	6
· Describe simulation study using ADEMP structure with sufficient rationale for choices.	
· Structure graphical and tabular presentations to place performance of competing methods side-by-side.	
· Include Monte Carlo SE as an estimate of simulation uncertainty.	5.2
· Publish code to execute the simulation study including user-written routines.	8

Simulations for estimands

Simple example: consider three estimators for mean μ of a distribution based on iid draws $Y_1 \ldots Y_n$: - θ_1: sample mean - θ_2: sample 20% trimmed mean - θ_3: sample median

If the distribution is symmetric, all three estimators should estimate the mean - If the distribution is skewed, they will give different answers

Simulations for estimands

For a particular choice of μ, n, and true underlying distribution:

- Generate independent draws $Y_1 \ldots Y_n$ from the distribution
- Compute θ_1, θ_2, θ_3 and repeat n_{sim} times to get:
  - $\theta_{1,1}, \ldots, \theta_{1,n_{sim}}$
  - $\theta_{2,1}, \ldots, \theta_{2,n_{sim}}$
  - $\theta_{3,1}, \ldots, \theta_{3,n_{sim}}$

Simulations for estimands

For $k = 1, 2, 3$, compute:

- $\hat{E}[\hat{\theta}_k]$
- $\widehat{bias}(\hat{\theta})$
- $\widehat{Var}(\hat{\theta})$
- $\widehat{coverage}(\hat{\theta})$

1. What is the estimand(s)?
2. What is the estimator(s)?
3. What is the performance measure(s)?

Simulations for hypothesis tests

Consider a t-test for whether the mean is equal to a specified value:

$$H_0 : \mu = \mu_0 \text{ vs. } H_1 : \mu \neq \mu_0$$

Suppose we want to evaluate whether the size/level of test achieves the advertised α. We would:

- Generate data under the **null hypothesis** and calculate proportion of rejections of H_0.
- This approximates Pr(reject H_0| H_0 true)
    - Should be $\approx \alpha$ if the method works well

Simulations for hypothesis tests

Suppose we want to evaluate **power**. We would:

- Generate data under some value of the alternative hypothesis $\mu \neq \mu_0$ and calculate proportion of rejection of H_0
- Approximates power, or Pr(reject $H_0 |\ H_1$ true)

Simulations for hypothesis tests

Size/level

```
set.seed(125)
nsim = 10000; n = 20; sigma = sqrt(5/3)
mu0 = 1
# Generate data from null distribution:
dat = matrix (rnorm (n*nsim, mu0, sigma), ncol=nsim, byrow=T)
opmean = apply (dat, 2, mean)
ses = sqrt(apply(dat, 2, var)/n)
tstats = (opmean - mu0)/ses
t05 = qt (0.975, n-1)
type1 = sum (abs (tstats) > t05)/nsim
type1
```

Simulations for hypothesis tests

Power

```
set.seed(125)
nsim = 10000; n = 20; sigma = sqrt(5/3)
mu0 = 1
mu = 1.85 ## Generate data from alternative
dat = matrix (rnorm (n*nsim, mu, sigma), ncol=nsim, byrow=T)
opmean = apply (dat, 2, mean)
ses = sqrt(apply(dat, 2, var)/n)
tstats = (opmean - mu0)/ses
t05 = qt (0.975, n-1)
power = sum (abs (tstats) > t05)/nsim
power
```

Setting the seed

Simulations use pseudo-random numbers generated by a random number generating algorithm

Each random number is a deterministic function of the current *state* of the random number generator

- After a random number is produced, the state changes, ready to produce next random number
- State is set using a **seed**
    - After enough random draws, the state will eventually repeat (the path is circular)

Setting the seed ensures **reproducibility** of the simulation results.

Setting the seed

How do you typically set the seed?

Setting the seed

Morris et. al. recommends setting seed *once per simulation scenario*

- All n_{sim} simulated datasets will be generated with the same seed
- Avoids potential non-independence in simulated datasets

A simple simulation study shows that using sequential seeds for each dataset is a problem in Stata:

$$x_1 = (0.1338766, 0.1364070, 0.4512149, \mathbf{0.0210242})$$
$$x_2 = (0.1364070, 0.4512149, \mathbf{0.0210242}, 0.3508981)$$
$$x_3 = (0.4512149, \mathbf{0.0210242}, 0.3508981, 0.9113581)$$
$$x_4 = (\mathbf{0.0210242}, 0.3508981, 0.9113581, 0.4707521).$$

Setting the seed

Using sequential seeds for each dataset appears to be less of a problem in R:

```
nobs = nsim = 4
set.seed(2025) # Morris approach
for(i in 1:nsim){
  # set.seed(i) # common approach
  print(runif(nobs))
}
```

Setting the seed

Morris et. al. recommends setting seed *once per simulation scenario*

- In practice this is often unrealistic
  - Simulation code is often run in parallel or on a cluster
  - *Common approach is to set seed for each simulated dataset*

```r
nobs = nsim = 4
# set.seed(2025) # Morris approach
for(i in 1:nsim){
  set.seed(i) # common approach
  print(runif(nobs))
}
```

Setting the seed, best practices

- *Common approach is to set seed for each simulated dataset*
  - Best practice for this approach is to draw a random seed

```
nobs = nsim = 3
seeds = sample(1:10000, nsim)
print(seeds)
for(i in 1:nsim){
  # set.seed(i) # common approach
  set.seed(seeds[i]) # slightly better approach
  print(runif(nobs))
}
```

Setting the seed, best practices

- Do not set the seed again later in the program, even if the methods being used have a stochastic component
- When writing functions and R packages, **do not hard code** a certain seed into the function/package
    - In fact, don't set a seed in the function or package at all, leave that up to the user

Monte Carlo standard errors

Monte Carlo standard errors quantify simulation uncertainty: they provide an estimate of the SE of (estimated) performance due to using finite n_{sim}

Performance Measure	Definition	Estimate	Monte Carlo SE of Estimate
Bias	$\mathrm{E}[\hat{\theta}] - \theta$	$\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}\hat{\theta}_i - \theta$	$\sqrt{\frac{1}{n_{\text{sim}}(n_{\text{sim}}-1)}\sum_{i=1}^{n_{\text{sim}}}(\hat{\theta}_i - \bar{\theta})^2}$
EmpSE	$\sqrt{\mathrm{Var}(\hat{\theta})}$	$\sqrt{\frac{1}{n_{\text{sim}}-1}\sum_{i=1}^{n_{\text{sim}}}(\hat{\theta}_i - \bar{\theta})^2}$	$\frac{\widehat{\mathrm{EmpSE}}}{\sqrt{2(n_{\text{sim}}-1)}}$
Relative % increase in precision (B vs A) [a]	$100\left(\frac{\mathrm{Var}(\hat{\theta}_A)}{\mathrm{Var}(\hat{\theta}_B)} - 1\right)$	$100\left(\left(\frac{\widehat{\mathrm{EmpSE}}_A}{\widehat{\mathrm{EmpSE}}_B}\right)^2 - 1\right)$	$200\left(\frac{\widehat{\mathrm{EmpSE}}_A}{\widehat{\mathrm{EmpSE}}_B}\right)^2\sqrt{\frac{1-\mathrm{Corr}(\hat{\theta}_A,\hat{\theta}_B)^2}{n_{\text{sim}}-1}}$
MSE	$\mathrm{E}[(\hat{\theta} - \theta)^2]$	$\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}(\hat{\theta}_i - \theta)^2$	$\sqrt{\frac{\sum_{i=1}^{n_{\text{sim}}}\left[(\hat{\theta}_i-\theta)^2-\widehat{\mathrm{MSE}}\right]^2}{n_{\text{sim}}(n_{\text{sim}}-1)}}$
Average ModSE[a]	$\sqrt{\mathrm{E}[\widehat{\mathrm{Var}}(\hat{\theta})]}$	$\sqrt{\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}\widehat{\mathrm{Var}}(\hat{\theta}_i)}$	$\sqrt{\frac{\widehat{\mathrm{Var}}[\widehat{\mathrm{Var}}(\hat{\theta})]}{4n_{\text{sim}}\times\widehat{\mathrm{ModSE}}^2}}$ [b]
Relative % error in ModSE[a]	$100\left(\frac{\mathrm{ModSE}}{\mathrm{EmpSE}} - 1\right)$	$100\left(\frac{\widehat{\mathrm{ModSE}}}{\widehat{\mathrm{EmpSE}}} - 1\right)$	$100\left(\frac{\widehat{\mathrm{ModSE}}}{\widehat{\mathrm{EmpSE}}}\right)\sqrt{\frac{\widehat{\mathrm{Var}}[\widehat{\mathrm{Var}}(\hat{\theta})]}{4n_{\text{sim}}\times\widehat{\mathrm{ModSE}}^4} + \frac{1}{2(n-1)}}$
Coverage	$\Pr(\hat{\theta}_{\text{low}} \le \theta \le \hat{\theta}_{\text{upp}})$	$\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}1(\hat{\theta}_{\text{low},i} \le \theta \le \hat{\theta}_{\text{upp},i})$	$\sqrt{\frac{\widehat{\mathrm{Cover.}}\times(1-\widehat{\mathrm{Cover.}})}{n_{\text{sim}}}}$
Bias-eliminated coverage	$\Pr(\hat{\theta}_{\text{low}} \le \bar{\theta} \le \hat{\theta}_{\text{upp}})$	$\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}1(\hat{\theta}_{\text{low},i} \le \bar{\theta} \le \hat{\theta}_{\text{upp},i})$	$\sqrt{\frac{\widehat{\text{B-E Cover.}}\times(1-\widehat{\text{B-E Cover.}})}{n_{\text{sim}}}}$
Rejection % (power or type I error)	$\Pr(p_i \le \alpha)$	$\frac{1}{n_{\text{sim}}}\sum_{i=1}^{n_{\text{sim}}}1(p_i \le \alpha)$	$\sqrt{\frac{\widehat{\mathrm{Power}}\times(1-\widehat{\mathrm{Power}})}{n_{\text{sim}}}}$

Number of simulations

How many simulated datasets do you need to capture the true sampling distribution of your estimator?

- Often this is chosen arbitrarily
  - $n_{sim} = 50, 100$ chosen to evaluate bias
  - $n_{sim} = 500, 1000$ chosen to evaluate coverage

Are these values large enough?

Number of simulations

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  - $n_{sim} = 50, 100$ chosen to evaluate bias
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Are these values large enough?

- each simulated dataset yields a draw from the true sampling distribution of the estimator, so n_{sim} is the "**sample size**" on which Monte Carlo estimates of the mean, bias, SD, etc are based

Number of simulations (bias)

Let's say we are interested in the **bias** of an estimator θ (whose true value is θ_0.)

Number of simulations (bias)

Let's say we are interested in the **bias** of an estimator θ (whose true value is θ_0.)

- True bias: $bias(\hat{\theta}) = E(\hat{\theta}) - \theta_0$
- Estimated bias: $\widehat{bias(\hat{\theta})} = \frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} \hat{\theta}_i - \theta_0$
- True variance: $Var(\hat{\theta}) = E\left[(\hat{\theta} - \theta_0)^2\right]$
- Estimated variance: $\widehat{Var(\hat{\theta})} = \frac{1}{n_{sim}-1} \sum_{i}^{n_{sim}} (\hat{\theta}_i - \bar{\theta})^2$

Number of simulations (bias)

Derive the Monte Carlo standard error of $\widehat{bias(\hat{\theta})}$

$$SE\left(\widehat{bias(\hat{\theta})}\right) = \sqrt{Var\left(\widehat{bias(\hat{\theta})}\right)} = \sqrt{Var\left(\frac{1}{n_{sim}}\sum_{i=1}^{n_{sim}} \hat{\theta}_i - \theta_0)\right)}$$

$$= \sqrt{\frac{1}{n_{sim}(n_{sim}-1)}\sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \bar{\theta})^2}$$

$$= \frac{\sqrt{\widehat{Var(\hat{\theta})}}}{\sqrt{n_{sim}}}$$

Number of simulations (bias)

To ensure our estimate of the bias has an acceptable amount of Monte Carlo standard error e, we can set

$$\frac{\sqrt{\widehat{Var(\hat{\theta})}}}{\sqrt{n_{sim}}} = e$$

Solving for n_{sim} gives:

$$n_{sim} = \frac{\widehat{Var(\hat{\theta})}}{e^2}$$

Can guess $\widehat{Var(\hat{\theta})}$ from prior knowledge or preliminary runs.

Number of simulations (coverage)

Coverage is the probability that a confidence interval contains θ.

- If α is set to 0.05, estimated coverage should be about 0.95 if a method is performing well
- Common performance measure for an estimator for θ

The Monte Carlo standard errors for coverage are

$$SE\left(\widehat{coverage}(\hat{\theta})\right) = \frac{\sqrt{\widehat{cover}(1 - \widehat{cover})}}{\sqrt{n_{sim}}}$$

Number of simulations (coverage)

Rearranging the previous equation, we get

$$n_{sim} = \frac{\widehat{cover}(1 - \widehat{cover})}{\left(SE(\widehat{coverage}(\hat{\theta}))\right)^2}$$

Let's assume $\alpha = 0.05$ and we want the Monte Carlo SE to be no more than 0.5% (.005):

$$n_{sim} = \frac{0.95(1 - 0.95)}{(0.005)^2} = 1900$$

Presenting your results

- **Key principle**: your simulation is useless unless other people (and your future self) can clearly understand what you did, why you did it, and what it means

Presenting the results

- **Key principle**: your simulation is useless unless other people can clearly understand what you did, why you did it, and what it means
- Before giving results, you must give the reader enough information to appreciate them.
  - State the objectives: Why do this simulation? What specific questions are you trying to answer?
  - State the **rationale** for choice of factors studied, assumptions made
  - Review all methods under study – be precise and detailed
  - Describe exactly how you generated data for each choice of factors. Enough detail should be given so that a reader could write his/her own program to reproduce your results

Presenting the results

- Results must be presented in a form that:
    - Clearly answers the questions
    - Makes it easy to appreciate the main conclusions
- Some basic principles:
    - Only present a subset of results ("Results were qualitatively similar for all other scenarios we tried.")
    - Only present information that is interesting ("Relative biases for all estimators were less than 2% under all scenarios and hence are not shown in the table.")
    - The mode of presentation should be friendly...

Presenting the results

- **Tables** are an obvious way to present results, however, some caveats:
  - Would a figure be more clear/compelling?
  - Place things to be compared adjacent to one another

Simple example: consider three estimators for mean μ of a distribution based on iid draws $Y_1 \ldots Y_n$: - θ_1: sample mean - θ_2: sample 20% trimmed mean - θ_3: sample median

Presenting the results

What's bad about this table?

	Sample	Mean	Trimmed	Mean	Median	
	Normal	t_5	Normal	t_5	Normal	t_5
Mean	0.98515	0.98304	0.98690	0.98499	0.99173	0.98474
Bias	-0.01485	-0.01696	-0.01310	-0.01501	-0.00827	-0.01526
SD	0.33088	0.33067	0.34800	0.31198	0.39763	0.35016
MSE	0.10959	0.10952	0.12116	0.09746	0.15802	0.12273

Presenting the results

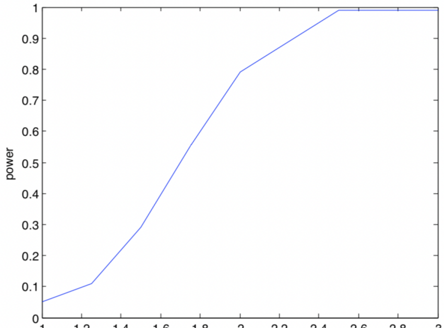
Improved version

	Normal			t_5		
	Sample Mean	Trim Mean	Median	Sample Mean	Trim Mean	Median
Mean	0.99	0.99	0.99	0.98	0.98	0.98
Bias	-0.01	-0.01	-0.01	-0.02	-0.02	-0.02
SD	0.33	0.35	0.40	0.33	0.31	0.35
MSE	0.11	0.12	0.16	0.11	0.10	0.12

Presenting the results

- Graphs/figures are often more effective than tables
- Example: Power of the t-test for $H_0 : \mu = 1$ vs. $H_1 : \mu \neq 1$ for normal data with $n_{sim} = 10000$, $n = 15$

μ	1.0	1.25	1.50	1.75	2.00	2.50	3.00
power	0.05	0.11	0.29	0.55	0.79	0.99	0.99



Final Takeaways

- **Principle 1**: A Monte Carlo simulation is just like any other experiment and requires planning
  - Can use experimental design principles
  - Shouldn't only choose factors favorable to a method you developed
  - n_{sim} should be chosen to achieve acceptable precision

Final Takeaways

- **Principle 2**: Save everything often!
  - Save the individual estimates in a file and then compute the mean, bias, SD, etc. later, as opposed to computing these summaries and saving only them
  - This is especially critical if the simulation takes a long time to run
  - Don't wait until the simulation ends to save. Long tasks can often be interrupted.

Final Takeaways

- **Principle 3**: Keep n_{sim} small at first
  - Test and refine code until you are sure everything is working correctly before carrying out final production runs
  - Get an idea of how long it takes to process one data set, i.e., one iteration
  - Particularly important if production run will be submitted to the cluster to determine how many cores may be necessary to finish in an acceptable time frame.

Final Takeaways

- **Principle 4**: Keep everything as reproducible as possible
  - Set and record the seed
  - Document your code!! Should be readable to your peer or your future self
  - Backup your code and results

References

[1] A. Burton, D. G. Altman, P. Royston, et al. "The design of simulation studies in medical statistics". In: *Statistics in medicine* 25.24 (2006), pp. 4279-4292.

[2] N. Metropolis. "THE BEGINNING of the Monte Carlo Method". In: *Los Alamos Science* 15 (1987), pp. 125-30.

[3] T. P. Morris, I. R. White, and M. J. Crowther. "Using simulation studies to evaluate statistical methods". In: *Statistics in medicine* 38.11 (2019), pp. 2074-2102.

Extra

Allowing for failures

Anticipate and **allow for failures** in a given simulation run. These can be do to:

- Rare events (e.g., assigned all subjects to a single treatment by chance, treatment perfectly confounded by a covariate in a permutation test)
- Lack of convergence of an optimization routine (fairly common in logistic regression)

Discard the failed iteration and repeat with the next random state but **record the number of failures** that occur to gauge how likely failure is in practice

Allowing for failures

To handle errors and other conditions in R

- `try()`: execution will continue when an error occurs
- `tryCatch()`: allows you to specify handler functions that give the computer directions about how to proceed when a condition is encountered

Allowing for failures

This will throw an error:

```
f1 = function (x){
  log(x)
}


f1("x")
# Error in log(x) : non-numeric argument to
# mathematical function
```

Allowing for failures

Using `try()` avoids failure:

```
f1 = function (x){
  try(log(x))
}


f1("x")
```

- Will print the error encountered during the `try()` statement, but doesn't break your code
- Using option `silent=TRUE` will suppress the message

Allowing for failures

In addition to handling errors, `tryCatch()` allows you to specify how to proceed in the event of a warning, message, or **interrupt**

- An interrupt is raised when the user terminates the program execution by pressing Ctrl+C (or similar).

```
result <- tryCatch(
  10 / "5",  # Code that might cause an error
  error = function(e) {
    message("Caught an error: ", e$message)
    return(NA)
  }
```