

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 2/4 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?

Motivation

- 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. ULM
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

They also look at 100 papers published in Statistics in Medicine and critique the design of the simulation studies.

ADEMP Structure

Aims	3.1
· Identify <i>specific</i> 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 i th 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 i th repetition
α	the nominal significance level
p_i	the p-value returned by the i th repetition

Estimands

What is an estimand?

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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 potential 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 $n \rightarrow \infty$, $\hat{\theta} \rightarrow \theta$
 - 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
 - Computational efficiency

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
<i>Analysis</i>		
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
<i>Design</i>		
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: $E[\hat{\theta}] - \theta$
 - used for estimands
- coverage: $Pr(\hat{\theta}_{low} \leq \theta \leq \hat{\theta}_{high})$
 - 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.
- Publish code to execute the simulation study including user-written routines.

5.2

8

Simulations for estimands

Simple example: consider three estimators for mean μ of a distribution based on iid draws $Y_1 \dots Y_n$:

- 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 $Y_1 \dots Y_n$ from the distribution
- Compute $\theta_1, \theta_2, \theta_3$ and repeat n_{sim} times to get:
 - $\theta_{1,1}, \dots, \theta_{1,n_{sim}}$
 - $\theta_{2,1}, \dots, \theta_{2,n_{sim}}$
 - $\theta_{3,1}, \dots, \theta_{3,n_{sim}}$

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 $\Pr(\text{reject } H_0 | H_0 \text{ true})$
 - 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 $\Pr(\text{reject } H_0 \mid H_1 \text{ true})$

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=TRUE)

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
```

```
[1] 0.7963
```

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

Setting the seed

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

- 4 datasets generated with `nsim = nobs = 4`, use seed 1:4 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*

```
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

Number of simulations

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

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- 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

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

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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

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	$E[\hat{\theta}] - \theta$	$\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \theta)$	$\sqrt{\frac{1}{n_{sim}(n_{sim}-1)} \sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \bar{\theta})^2}$
EmpSE	$\sqrt{Var(\hat{\theta})}$	$\sqrt{\frac{1}{n_{sim}-1} \sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \bar{\theta})^2}$	$\frac{EmpSE}{\sqrt{2(n_{sim}-1)}}$
Relative % increase in precision (B vs A)*	$100 \left(\frac{Var(\hat{\theta}_A)}{Var(\hat{\theta}_B)} - 1 \right)$	$100 \left(\left(\frac{EmpSE_A}{EmpSE_B} \right)^2 - 1 \right)$	$200 \left(\frac{EmpSE_A}{EmpSE_B} \right)^2 \sqrt{\frac{1 - Corr(\hat{\theta}_A, \hat{\theta}_B)}{n_{sim}-1}}$
MSE	$E[(\hat{\theta} - \theta)^2]$	$\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \theta)^2$	$\sqrt{\frac{\sum_{i=1}^{n_{sim}} [(\hat{\theta}_i - \theta)^2 - MSE]^2}{n_{sim}(n_{sim}-1)}}$
Average ModSE*	$\sqrt{E[Var(\hat{\theta})]}$	$\sqrt{\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} Var(\hat{\theta}_i)}$	$\sqrt{\frac{Var[Var(\hat{\theta})]}{4n_{sim} \times ModSE}} \quad b$
Relative % error in ModSE*	$100 \left(\frac{ModSE}{EmpSE} - 1 \right)$	$100 \left(\frac{ModSE}{EmpSE} - 1 \right)$	$100 \left(\frac{ModSE}{EmpSE} \right) \sqrt{\frac{Var[ModSE]}{4n_{sim} \times ModSE^2} + \frac{1}{2(n-1)}}$
Coverage	$Pr(\hat{\theta}_{low} \leq \theta \leq \hat{\theta}_{upp})$	$\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} I(\hat{\theta}_{low,i} \leq \theta \leq \hat{\theta}_{upp,i})$	$\sqrt{\frac{Cover \times (1 - Cover)}{n_{sim}}}$
Bias-eliminated coverage	$Pr(\hat{\theta}_{low} \leq \bar{\theta} \leq \hat{\theta}_{upp})$	$\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} I(\hat{\theta}_{low,i} \leq \bar{\theta} \leq \hat{\theta}_{upp,i})$	$\sqrt{\frac{B-E \times Cover \times (1 - B-E \times Cover)}{n_{sim}}}$
Rejection % (power or type I error)	$Pr(p_i \leq \alpha)$	$\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} I(p_i \leq \alpha)$	$\sqrt{\frac{Power \times (1 - Power)}{n_{sim}}}$

Number of simulations (bias)

Let's say we are interested in the **bias** of an estimator $\hat{\theta}$ (whose true value is θ_0 .)

Number of simulations (bias)

Let's say we are interested in the **bias** of an estimator $\hat{\theta}$ (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: $Var(\hat{\theta}) = E[(\hat{\theta} - \theta_0)^2]$
- 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 $\widehat{bias}(\hat{\theta})$

$$\begin{aligned} SE\left(\widehat{bias}(\hat{\theta})\right) &= \sqrt{Var\left(\widehat{bias}(\hat{\theta})\right)} = \sqrt{Var\left(\frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} \hat{\theta}_i - \theta_0\right)} \\ &= \sqrt{\frac{1}{n_{sim}(n_{sim}-1)} \sum_{i=1}^{n_{sim}} (\hat{\theta}_i - \bar{\theta})^2} \\ &= \frac{\sqrt{\widehat{Var}(\hat{\theta})}}{\sqrt{n_{sim}}} \end{aligned}$$

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

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

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

- 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 $Y_1 \dots Y_n$:

- 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

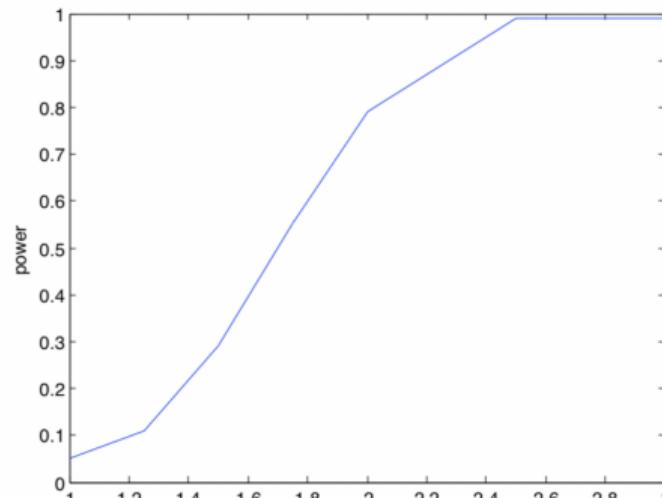
Improved version

	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

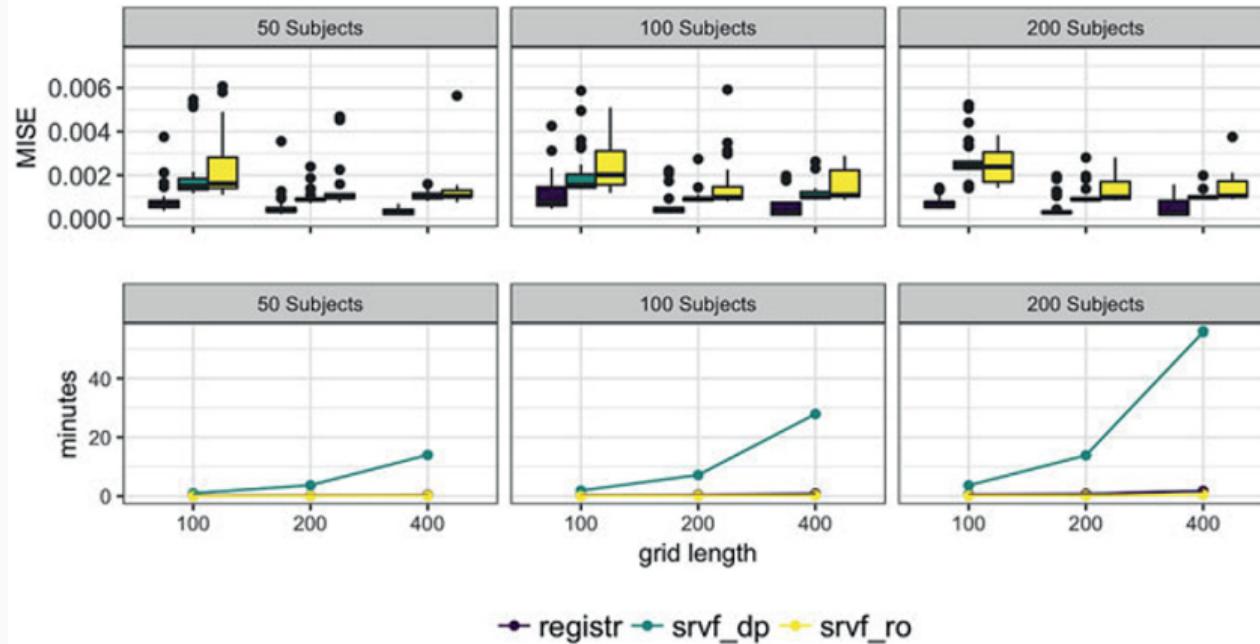
Presenting the results

- 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



Presenting the results



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

- Use the results to judge whether the statistical procedure can reliably be used in the situation(s) being investigated

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)  
  }  
)  
  
print(result)
```