



Coding robust simulation studies in Stata

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Smarter Studies Global Impact Better Health

Plan of talk

Introduce simulation studies and **ADEMP**

Some tips when something has gone wrong

Analysis of simulation studies using siman



Introducing simulation studies

Simulation studies are used in a variety of disciplines.

They are an important and useful tool which enables researchers to compare different statistical methods and understand their properties.



What can simulation studies be used for?

- Check that code does the intended analysis
- Check robustness of programs
- Better understand statistical concepts
- Understand new commands
- Check algebra
- Evaluate a new statistical method
- Compare statistical methods head-to-head
- Calculate sample size / power
- ...and more



Simulation study set up: ADEMP

In a simulation study, data is often generated from some distribution (so often we know the truth), the data is analysed and compared with the known truth. Convenient to plan using 'ADEMP' structure.

Aims: What question(s) the simulation study addresses Data-generating mechanisms (DGMs): How the simulated datasets are to be generated Estimands/targets: quantities to be estimated by the analysis Methods of analysis: How a given simulated dataset is to be analysed Performance measures: How the performance of the methods of analysis is to be summarised

(Also worth thinking about implementation and reporting)





Two types of dataset

	344									
rep_no 1	×1 16.35013	x2 1	У 38.37179				rep_no	theta		se
1	24.2343	- 0	34.14901				1	.7253602		113077
1	3. rep_no	x1	x2	У			2	.9061058	1 1	571631
1	8.	2 23.866	39 0	47.72385						
1	12	2 26.775	22 1	58.26255			3	-2.685881	.34	420264
1	23	2 rep_no	x1	x2	У		4	-1.277903	.4	767973
1	17	2	3 17.67529	1	49.35355					492868
1	3.	2	3 10.84167	0	58.08726		Feti	imate	c	418173
1		າ _	9807		47.08185		LSU	mate		
1	Sim	ulat	ed 5374		56.96053		dat	aset		879704
1			9691		50.6784		ual	asei	4	439402
1	data	aset	S 6223		64.59888		9	.2409494	.34	497852
1					42.93995		10	-1.188984		
1			3 26.54299 3 23.86617		50.52908 47.02399		10	-1.100904	.0	971455
1			3 23.86617 3 11.20086		47.83489		11	1022815	.0	010391
1			3 12.41312		62.99809		12	6783351	. 20	035454
1			3 29.38236		51.41874		13	-2.006534	.0	005921
1	.9	2	3 14.01399	0	65.50615					
1	23	2	3 10.74801	. 0	52.5156		14	3832266	.0	561816
		2	3 21.1476	; 1	55.21921		15	-1.33277	.0	143398
	1	2	3 16.47218	0	49.29565		16	5361734	.8	849165
		2	3 14.00056	; 1	54.68225		17	1.535977	. 3	798626
			3 16.78905	; 1	61.35783					
			3 3.979811	. 0	44.87682		18	1.089039	.5	508905
			3 2.89212	1	62.30411		19	-1.446115	.1	594974

20 -.6660534

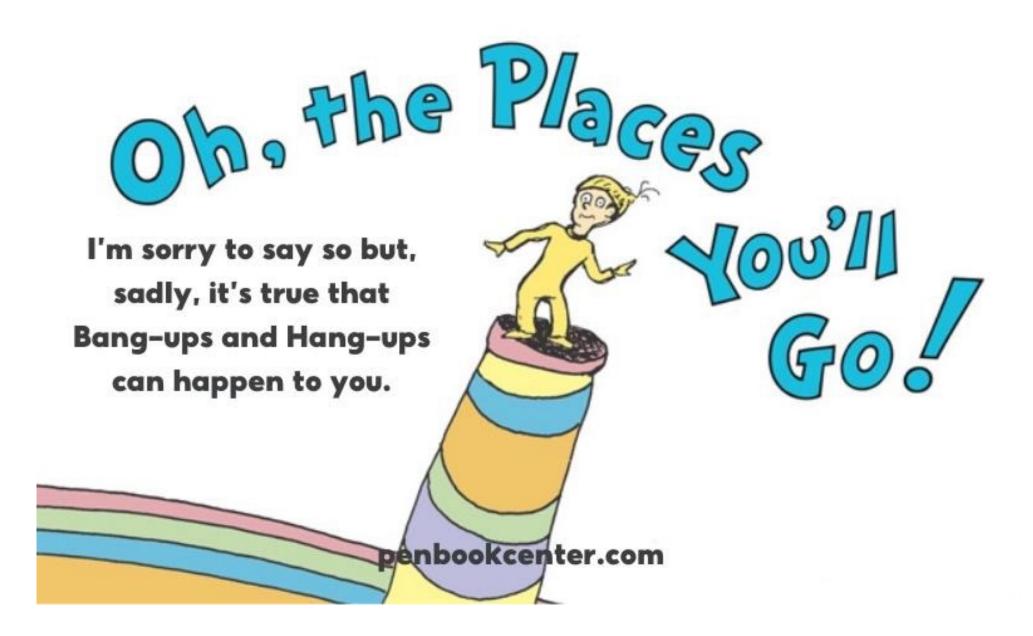
.7300485

I don't believe it!

We often find ourselves in the position of seeing some simulation results – our own, a colleague's or a student's – and thinking:

'I'M SCEPTICAL OF THESE RESULTS' or **'I DON'T BELIEVE THIS'**





But is it wrong?

The fact that we are sceptical does not necessarily mean the result is wrong

That being said, in many cases it is.

We need to make sure we have exhausted possible errors to the extent possible.



Three 'phases' of simulation study







Design Getting ADEMP right!

Conduct

Writing code to generate data, analyse, store results

Analysis

Computing performance measures from an estimates dataset



A series of tips

Based on 'How to check a simulation study' osf.io/cbr72/ (pre-print).

Problems often arise when we have many DGMs, estimands and/or methods of analysis.

Issues that involve Stata can occur in any of the three stages.



Running example: White & Carlin

Loosely based on: White IR, Carlin JB. Bias and efficiency of multiple imputation compared with complete-case analysis for missing covariate values. *Statistics in Medicine* 2010; 29: 2920–2931.



Running example: White & Carlin

Aim	To compare multiple imputation with complete case analysis.
Data-generating mechanism (rough)	Quantitative confounder C is drawn from a standard Normal distribution.
	Binary exposure E and binary outcome D are drawn from logistic models depending on C (so E does not cause D).
	Data are made missing on C, initially using a missing completely at random model.
	Parameters to be varied are the marginal probabilities of E and D, the strength of the dependence of E and D on C, and the missing data mechanism. The sample size of 500 is fixed.



Running example: White & Carlin

Estimand	The log odds ratio between E and D, conditional on C.						
Methods of analysis	1. Analysis of full data before data deletion in C.						
	2. Analysis of complete cases (excluding cases with missing C).						
	3. Multiple imputation of missing values of C (various imputation						
	models may be used).						
Performance measures	s Bias						
	Empirical standard error						
	Relative error in model-based standard error						
	Coverage						
Implementation?	1,000 repetitions						



Two tips

TIP: If possible, include a 'benchmark' setting with known properties – either known theoretically or 'known' from someone else's simulation study. In our missing data example, we have included 'full data' as this should give better performance than any analysis with incomplete data.

TIP: Write well-structured code *from the start!*



Well-structured code?

Two criteria for 'well structured code':

- 1. For a single repetition, to the extent possible, separate data generation, data analysis and 'posting'/storage of result/s
- 2. Produce a well-structured estimates dataset



Well structured code: a suggestion

Write:

- A program that generates data
- A program that analyses data and returns (or directly posts) results of interest
- A program that repeatedly calls these and structures the results sensibly an estimates dataset



DGM program

```
program define gendata
```

version 17

```
syntax, obs(int) logite(string) logitd(string) pmiss(string)
```

```
clear
```

```
set obs `obs'
```

drawnorm Ctrue

```
gen E = runiform() < invlogit(`logite')</pre>
```

```
gen D = runiform() < invlogit(`logitd')</pre>
```

```
gen Cobs = Ctrue if runiform()>=`pmiss'
```

end



Analysis program

```
program define anadata
```

```
version 14
syntax, rep(int 0) [ post(string) ]
```

```
* Method 1: full data before data deletion
logit D E Ctrue
if !mi("`post'") post `post' (`rep') ("Full") (_b[E]) (_se[E]) (e(N)) (.)
* we are posting: rep method est se N df
...
```

```
mi impute regress Cobs D##E, add(5)
mi estimate, post: logit D E Cobs
if !mi("`post'") post `post' (`rep') ("MI") (_b[E]) (_se[E]) (e(N)) ///
   (e(df_mi)[1,"D:E"])
```

end



Tip: study a single very large dataset

Ideally, 'fit back' the data-generating model and check that number of observations is correct, parameters are close to inputs, true values of parameters are trapped by confidence intervals, etc.

gendata , obs(100000)



Tip: run with three repetitions

- 1. Verify that your estimates dataset is 'well-structured'
- 2. Verify that the second and third repetitions produce different data and results

Why? Sometimes simulation code wrongly sets the seed within a program starting the first repetition. This is sometimes done in some program called by gendata or anadata.

If (for example) this is done at the end of a repetition, the second and third repetitions will produce identical data and results.



Tip: run with three repetitions

- . set rngstream 1
- . set seed 576819506
- . local nreps 3
- . tempname est
- . postfile `est' int(rep) str3(method) float(b se) int(N) float(df)
- > using estimates, replace
- . forvalues i=1/`nreps' {
- . gendata, obs(500) logite(-1+C) logitd(-1+C) pmiss(.3)
- . anadata, rep(`i') post(`est')
- }
- . postclose `est'



Tip: run with three repetitions

. list, sepby(rep)

-	+					+
	rep	method	b	se	Ν	df
1.	 1	Full	1081978	.2457296	500	·
2.	1	CCA	3064098	.314233	337	•
3.	1	MI	207532	.2880667	500	71.65478
4.	 2	 Full	.0867077	.2260111	500	
5.	2	CCA	.1381473	.2631429	349	.
6.	2	MI	.1110958	.2330245	500	1092.247
7.	 3	 Full	.1232898	.2289063	500	 .
8.	3	CCA	1608068	.2822033	348	•
9.	3	MI	.0335785	.2445695	500	508.5607
-	+					+





Tip: anticipate analysis failures

Code should be written to capture the error so the simulation does not halt.

The failure of a method should be stored – and investigated – along with its error code.

- . capture noisily logit D E Cobs
- . if _rc==0 & !mi("`post'") post `post' (`rep') ("CCA")
- > (_b[E]) (_se[E]) (e(N)) (.) (_rc)
- . if _rc>0 & !mi("`post'") post `post' (`rep') ("CCA") (.)
- > (.) (.) (.) (_rc)



Tip: make it easy to recreate any simulated dataset

Your estimates dataset needs a unique identifier for each result (I have a repetition number and a variable giving the method of analysis used)

If we can recreate a specific result, we can explore method failures, outliers, etc. Two ways:

- 1. Store the RNG state at the start of a repetition: see github.com/tpmorris/TheRightWay/
- 2. Save every simulated dataset (if the analysis has a stochastic element, such as multiple imputation or bootstrap, you still need the RNG state)



Analysis tips

The pre-print gives some tips for understanding issues with analysis, which we won't recap here (more focused on understanding results than on 'coding robust simulation studies').

If you have a well-structured estimates dataset, Ella is now going to talk through a suite of commands that analyse a simulation study. In particular, it automates unpleasant data wrangling, analysis and several graphics.



ELLA'S SLIDES



Introducing siman

We introduce the siman suite which has been created to assist the analysis of simulation results.

A set of Stata programs that offer data manipulation, analysis and graphics to process, explore and visualise the results of simulation studies.

The new siman program described here is available at *https://github.com/UCL/siman*

Work with Ian White and Tim Morris, MRC Clinical Trials Unit at UCL



Types of dataset: Estimates data

- Estimates data set: results from analysing multiple simulated data sets, with data relating to different statistics (e.g. point estimate (est), se) for each simulated data set.
- repetition (rep): simulation number

		rep	dgm	estimand	method	est	se	true	
	1	1	1	beta	А	1433122	.0773843	0	
	2	1	1	beta	В	23375	.1103629	0	
	3	1	1	gamma	А	051712	.0809558	0	
	4	1	1	gamma	В	1375358	.1166905	0	
	5	1	2	beta	А	1134563	.0945678	0	
	6	1	2	beta	В	1543437	.1399313	0	
	7	1	2	gamma	А	0597119	.0934798	0	
	8	1	2	gamma	В	1588126	.1347426	0	
	9	2	1	beta	А	1508732	.0768133	0	
	10	2	1	beta	В	0784156	.1087276	0	
	11	2	1	gamma	А	0296873	.0737869	0	
	12	2	1	gamma	В	.1310411	.1115952	0	
	13	2	2	beta	А	1337332	.0927938	0	
	14	2	2	beta	В	1540722	.1323587	0	
	15	2	2	gamma	А	0342799	.0852017	0	
Jnit	16	2	2	gamma	В	.1513133	.128859	0	



Types of dataset: long and wide

For the input estimates data, there are 3 formats permitted by the siman suite:

- 1. Long for both targets and methods: longlong
- 2. Wide for both target and methods : widewide
- 3. Long for targets, wide for methods : longwide

								rep	dgm	estimand	method	est	se	true		
					rep	dgm		estimand	estA	seA	estB	seB	true			
				1	1		1	beta	1433122	.0773843	23375	.1103629	0			
				2	1		1	gamma	051712	.0809558	1375358	.1166905	0			
			r	З	1		2	beta	1134563	.0945678	1543437	.1399313	0		seBgamma	true
	1	1		4	1		2	gamma	0597119	.0934798	1588126	.1347426	0		.1166905	0
	2	1		5	2		1	beta	1508732	.0768133	0784156	.1087276	0		.1347426	0
				6	2		1	gamma	0296873	.0737869	.1310411	.1115952	0			
MRC Clinical Trials Uni	3	2		7	2		2	beta	1337332	.0927938	1540722	.1323587	0		.1115952	0
	4	2		8	2		2	gamma	0342799	.0852017	.1513133	.128859	0		.128859	0
						9	2		1	beta	А	1508732	.0768133	0		
2 1 3 2 4 2					10	2		1	beta	В	0784156	.1087276	0			
					11	2		1	gamma	А	0296873	.0737869	0			
					12	2		1	gamma	В	.1310411	.1115952	0			
						13	2		2	beta	А	1337332	.0927938	0		
RC						14	2		2	beta	В	1540722	.1323587	0		
	al					15	2		2	gamma	А	0342799	.0852017	0		
						16	2		2	gamma	В	.1513133	.128859	0		

Performance Measures

Typically a statistical method outputs an estimate $\hat{\theta}$, its standard error $se(\hat{\theta})$ and a confidence interval ($\hat{\theta} low$, $\hat{\theta} upp$)

The following performance measures may be of interest:

- •Properties of estimate $\hat{\theta}$
 - ■Bias
 - Empirical SE
 - ■MSE
- Properties of SE
 - Average model-based SE
- •Properties of confidence interval
 - Coverage
 - Power



Types of Data Sets: OUTPUT Performance Measures

Performance measures data set: results from analysing an estimates data set, with data relating to different performance measures (e.g. bias, coverage) summarised over estimates data sets for different data generating mechanisms.

	rep	dgm	estimand	method	est	se	true	_perfmeascode	_dataset
1	Non-missing point estimates	1	beta	А	1000			bsims	Performance
2	Non-missing point estimates	1	beta	В	1000			bsims	Performance
з	Non-missing standard errors	1	beta	А	1000			sesims	Performance
4	Non-missing standard errors	1	beta	В	1000	-	-	sesims	Performance
5	Bias in point estimate	1	beta	А	0043991	.0024993		bias	Performance
6	Bias in point estimate	1	beta	В	0025973	.0035644		bias	Performance
7	Mean of point estimate	1	beta	А	0043991	.0024993		mean	Performance
8	Mean of point estimate	1	beta	В	0025973	.0035644		mean	Performance
9	Empirical standard error	1	beta	А	.0790336	.0017681		empse	Performance
10	Empirical standard error	1	beta	В	.1127159	.0025217		empse	Performance
11	% precision gain relative to method A	1	beta	А			-	relprec	Performance
12	% precision gain relative to method A	1	beta	В	-50.8353	2.28676		relprec	Performance
13	Mean squared error	1	beta	А	.0062594	.0002881	-	mse	Performance
14	Mean squared error	1	beta	В	.0126989	.0006187	-	mse	Performance
15	Root mean squared error	1	beta	А	.0791165	.0230148		rmse	Performance
16	Root mean squared error	1	beta	В	.1126895	.0243622	-	rmse	Performance
17	RMS model-based standard error	1	beta	А	.0787452	.0001572		modelse	Performance
18	RMS model-based standard error	1	beta	В	.1136343	.0003405		modelse	Performance
19	Mean conf. interval width	1	beta	А	.3080681	.0006123		ciwidth	Performance
20	Mean conf. interval width	1	beta	В	.4434751	.0013217		ciwidth	Performance
21	Relative % error in standard error	1	beta	А	3649609	2.237882		relerror	Performance
22	Relative % error in standard error	1	beta	В	.8147949	2.275551		relerror	Performance
23	% coverage of nominal 95% conf. interval	1	beta	А	94.7	.7084563		cover	Performance
24	% coverage of nominal 95% conf. interval	1	beta	В	95.7	.6414907		cover	Performance



Setting up siman: long-long format

siman setup takes the estimates data set held in memory, checks the data, reformats it if necessary and attaches characteristics to the data set available for use across multiple sessions.

	rep	dgm	estimand	method	est	se	true	
1	1	1	beta	А	1433122	.0773843	0	
2	1	1	beta	В	23375	.1103629	0	
3	1	1	gamma	А	051712	.0809558	0	
4	1	1	gamma	В	1375358	.1166905	0	
5	1	2	beta	А	1134563	.0945678	0	
6	1	2	beta	В	1543437	.1399313	0	
7	1	2	gamma	А	0597119	.0934798	0	
8	1	2	gamma	В	1588126	.1347426	0	
9	2	1	beta	А	1508732	.0768133	0	
10	2	1	beta	В	0784156	.1087276	0	
11	2	1	gamma	А	0296873	.0737869	0	
12	2	1	gamma	В	.1310411	.1115952	0	
13	2	2	beta	А	1337332	.0927938	0	
14	2	2	beta	В	1540722	.1323587	0	
15	2	2	gamma	А	0342799	.0852017	0	
16	2	2	gamma	В	.1513133	.128859	0	

siman setup, rep(rep) dgm(dgm) target(estimand) method(method) est(est) se(se) true(true)



MRC



Setting up siman: wide-wide format

	rep	dgm	estAbeta	seAbeta	estBbeta	seBbeta	estAgamma	seAgamma	estBgamma	seBgamma	true	
1	1	1	1433122	.0773843	23375	.1103629	051712	.0809558	1375358	.1166905	0	
2	1	2	1134563	.0945678	1543437	.1399313	0597119	.0934798	1588126	.1347426	0	
3	2	1	1508732	.0768133	0784156	.1087276	0296873	.0737869	.1310411	.1115952	0	
4	2	2	1337332	.0927938	1540722	.1323587	0342799	.0852017	.1513133	.128859	0	

siman setup, rep(rep) dgm(dgm) target(beta gamma)
method(A B) est(est) se(se) true(true) order(method)



Setting up siman: siman describe

SUMMARY OF DATA

The siman format is:	format 1: long-long
The format for targets is:	long
The format for methods is:	long
The number of targets is:	2
The target values are:	beta gamma
The number of methods is:	2
The method values are:	A B
Data generating mechanism (dgm) The total number of dgms is: The dgm variables (# levels): Estimates are contained in the da	2 dgm (2) ataset
The estimates variable is:	est
The se variable is:	se
The df variable is:	N/A
The ci variables are:	N/A
The p variable is:	N/A
The true variable is:	true



Exploring the estimates data: siman reshape

2 1 3 1 4 1 5 2 6 2 7 2 8 2	rep dgm		estimand	estA	se	4	estB	seB	tr	ue								
4 1 5 2 6 2 7 2 8 2	1	1	beta	1433122	.077	3843	23375	.11036	29	0								
	1	1	gamma	051712	.080	9558	1375358	.11669	05	0								
	1	2	beta	1134563	.094	5678	1543437	.13993	13	0								
	1	2	gamma	0597119	.093	4798	1588126	.13474	26	0								
	2	1	beta	1508732	.076	3133	0784156	.10872	76	0								
	2	1	gamma	0296873	.073	7869	.1310411	.11159	52	0								
	2	2	beta	1337332	.092	7938	1540722	.13235	87	0								
	2	2	gamma	0342799	.085	2017	.1513133	.1288	59	0								
			_				rep	dgm	estimand	method	est	se	true					
					1	1		1	beta	А	1433122	.0773843	0					
					2	1		1	beta	В	23375	.1103629	0					
					3	1		1	gamma	А	051712	.0809558	0					
					4	1		1	gamma	В	1375358	.1166905	0					
					5	1		2	beta	А	1134563	.0945678	0					
	l-		7	٦	6	1		2	beta	В	1543437	.1399313	0					
	an resh	iape,	Long	Long	7	1		2	gamma	А	0597119	.0934798	0					
	1.		-			1 ' .] .]	8	1		2	gamma	В	1588126	.1347426	0	
	an resh	nape,	Long	wide	9	2		1	beta	А	1508732	.0768133	0					
					10	2		1	beta	В	0784156	.1087276	0					
					11	2		1	gamma	А	0296873	.0737869	0					
					12	2		1	gamma	В	.1310411	.1115952	0					
					13	2		2	beta	А	1337332	.0927938	0					
					14	2		2	beta	В	1540722	.1323587	0					
					15	2		2	gamma	А	0342799	.0852017	0					
sima sima					16	2		2	gamma	В	.1513133	.128859	0					



Exploring the estimates data: example data from earlier

simcheck paper, White et al. (preprint <u>https://osf.io/cbr72/)</u>

							true dgm 0 2		
	rep	method	ь	se	df	true	dgm		
1	1	Full	3664537	.4296166		0	2		
2	1	CCA	6404278	.5808458	-	0	2		
З	1	MI	7200662	.4606918	1350.781	0	2		
4	2	Full	.4978587	.4003829	-	0	2		
5	2	CCA	.7493323	.4796979	-	0	2		
6	2	MI	.5480893	.4190439	527.496	0	2		
7	З	Full	0834949	.335249	-	0	2		
8	З	CCA	4181158	.4036536	-	0	2		
9	З	MI	2691882	.3600377	362.7664	0	2		
10	4	Full	4460969	.370079	-	0	2		
11	4	CCA	371215	.3978041	-	0	2		
12	4	MI	3969929	.3777045	1664.085	0	2		
13	5	Full	4702572	.3891214	-	0	2		
14	5	CCA	3799451	.4851103	-	0	2		
15	5	MI	4747566	.4262364	174.7589	0	2		
16	6	Full	.0816109	.385957	-	0	2		
17	6	CCA	1413643	.4341343	-	0	2		
18	6	MI	.0940165	.4007708	841.9497	0	2		



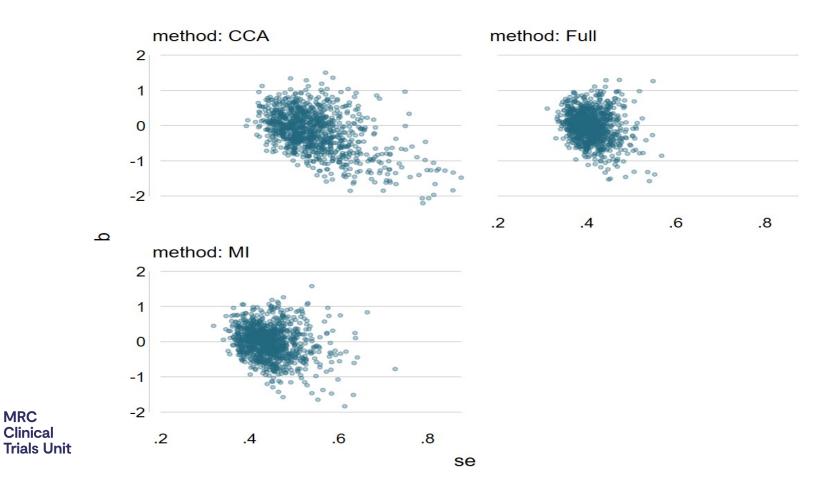
Trials L

Exploring the estimates data: siman scatter

siman scatter [if] [in] [, options]

siman scatter if dgm == 1

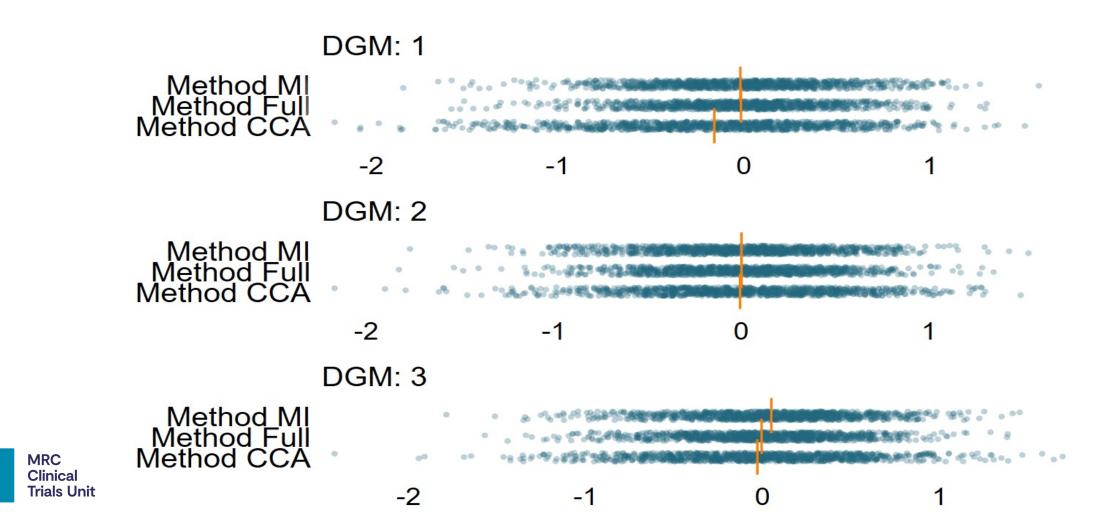
MRC



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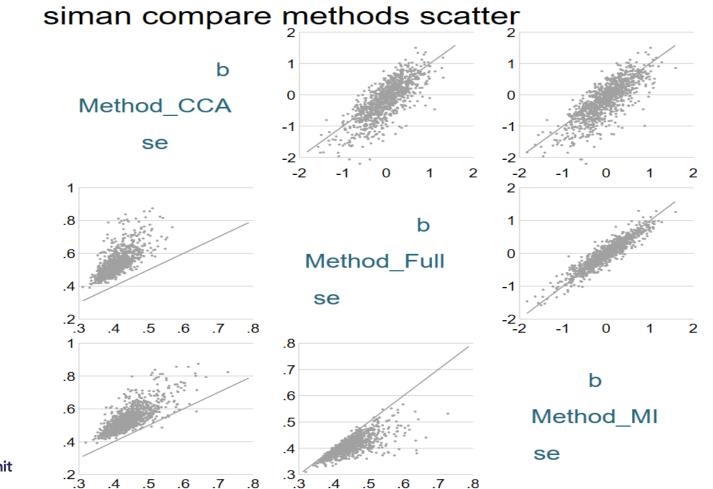
Exploring the estimates data: siman swarm

siman swarm [if] [in] [, options]



Exploring the estimates data: siman comparemethodsscatter

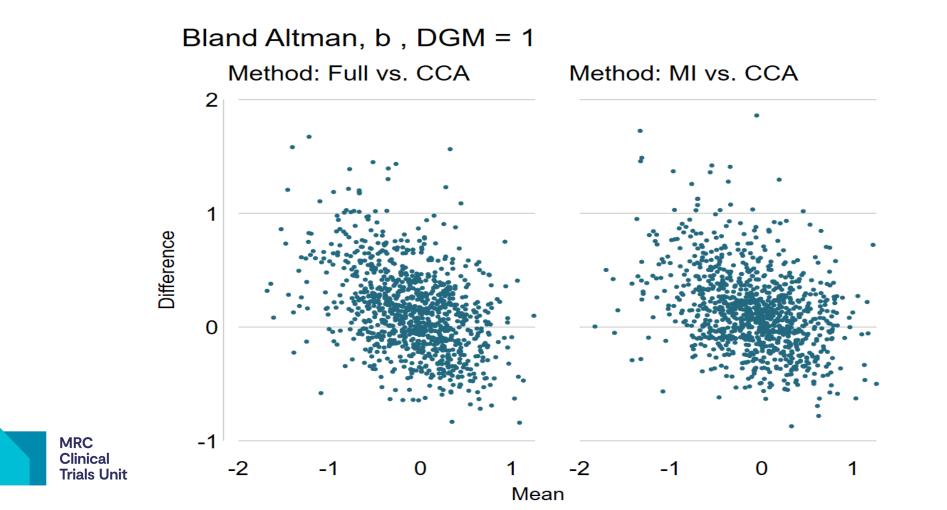
siman comparemethodsscatter [estimate|se] [if] [in] [, options]



MRC Clinical Trials Unit

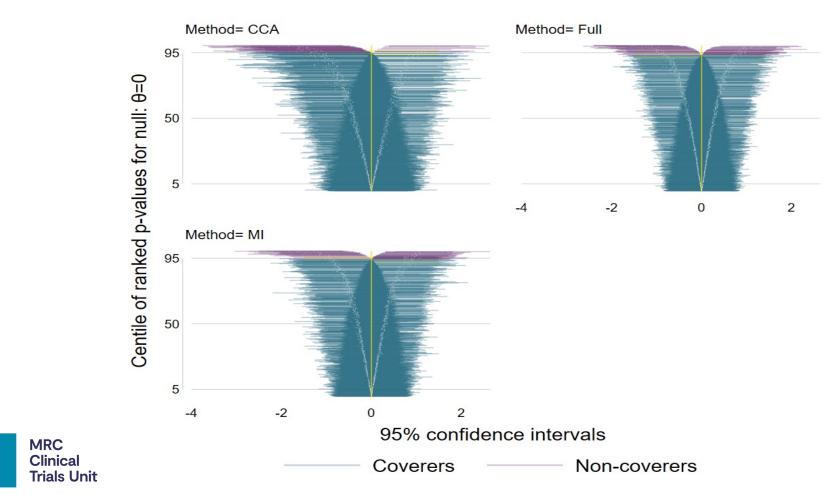
Exploring the estimates data: siman blandaltman

siman blandaltman [if] [in] [, options]



Exploring the estimates data: siman zipplot

siman zipplot [if] [in] [, options]



Creating performance measures

Once siman setup has been run, performance measures can be created using the command siman analyse

```
siman analyse [if], [performancemeasures perfonly
replace]
```

performancemeasures as per simsum. If none of the following options are specified, then all available performance measures are computed.....

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Creating performance measures cont.

perfonlythe program will automatically append theperformance measures data to the estimates data,
unless the user specifies perfonly for performance
measures only.

replaceif siman analyse has already been run and the userspecifies it again then they must use the replaceoption, to replace the existing performance measuresin the data set.



Creating performance measures: siman table

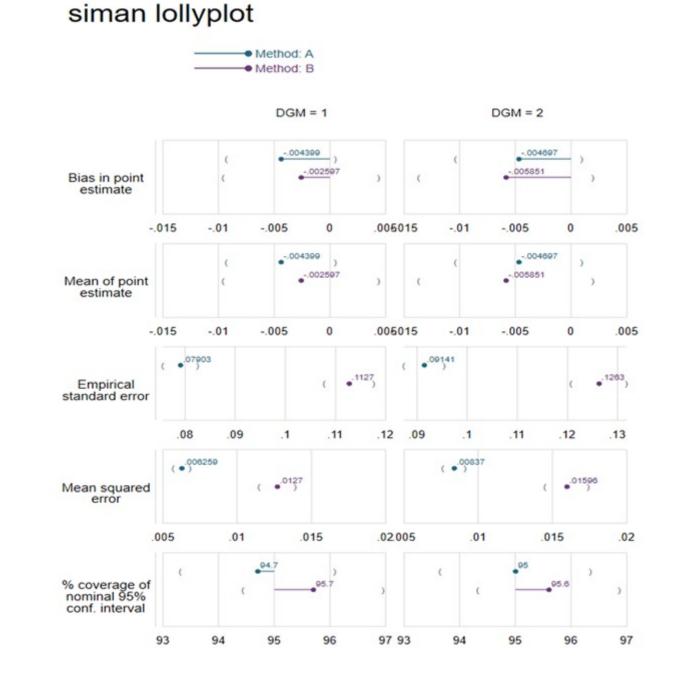
siman table [performancemeasures] [if], [column(varname)]
siman table bias

. siman table bias

method			dgm and performance
MI	Full	CCA	measure
			1
0203649	0168955	160113	bias
.0146205	.0137363	.0183634	
			2
.0000898	0000126	0075347	bias
.0143525	.0134727	.0163235	
			3
.0486318	0063853	0301532	bias
.0145317	.0136254	.0170389	



NOTE: Where there are 2 entries in the table, the first entry is the performance measure and the second entry is its Monte Carlo error.





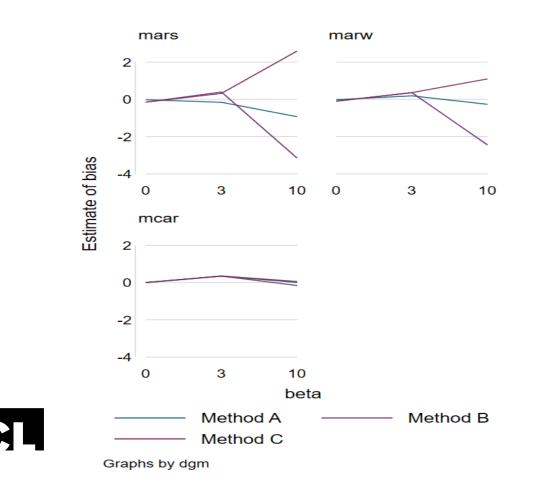
siman lolly



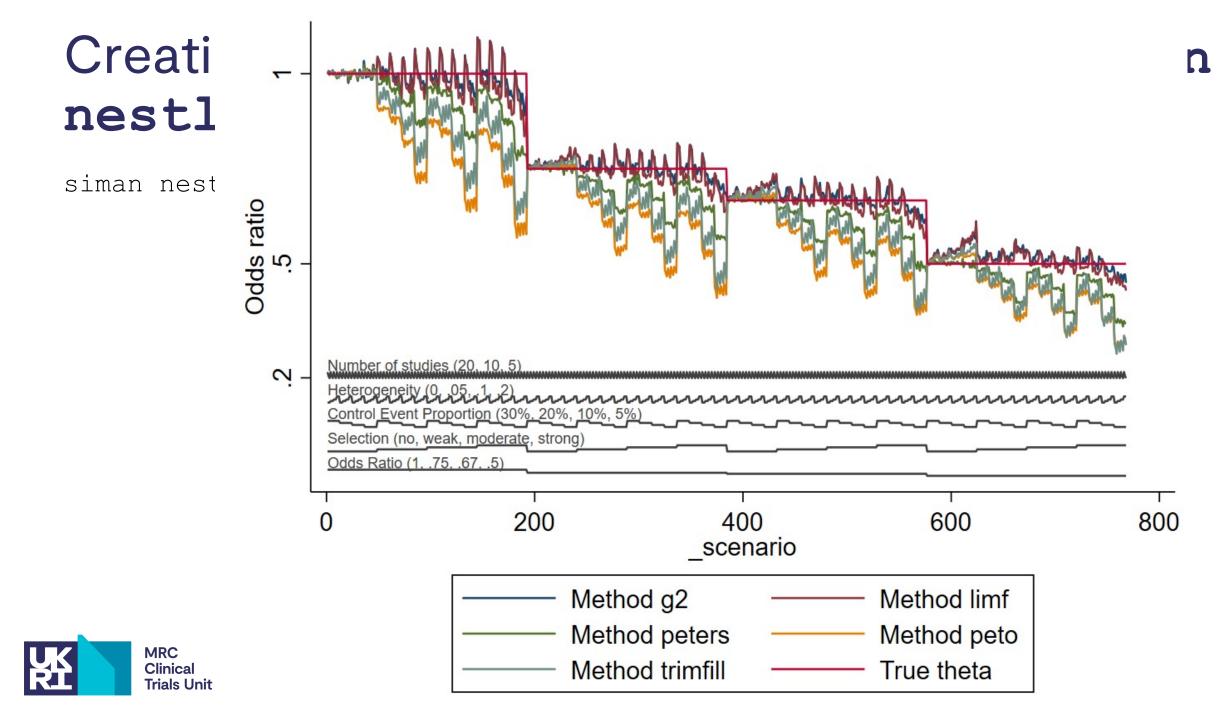
hs: siman

Creating performance measures graphs: siman trellis

siman trellis [performancemeasures] [if] [, options]







Software testing

We have a program of testing our unit's software.

The siman suite is being tested on numerous data set formats by EMZ, IW, TM: long-long, long-wide, wide-wide, numeric and string, multiple methods, targets and dgms.

Error checking to make sure it fails when it is meant to (with a sensible error message).



Roundup 1

We've given a collection of tips that help to find/avoid errors in simulation studies.

The siman suite automates the data wrangling and analysis that often leads to problems. People often, for example:

- 1. Tangle up DGMs with methods
- 2. Compute average of model SEs (instead of root-mean variance)
- 3. Forget to separate out different estimands, DGMs or methods



Roundup 2

Doing all these things may simply be a matter of reassuring yourself that a particular result is 'real' and not goofing the code.

One remaining (unpopular?) tip if you don't believe your results: write at least some of your code in another software package. In the pre-print, there is code for both Stata and R, and the different approaches to handling nearseparation are very interesting.



Acknowledgements





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Tra My Pham



Michael

Crowther



Jingyi Xuan



Matteo Quartagno 52

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