Design of Simulation Experiments

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Research Process of Simulation



See Barth/Meyer/Spitzner (2012): Typical Pitfalls of Simulation Modeling – Lessons learned from Business and Military, in: JASSS, 15, 2. Adpated from Railsback/Grimm (2012): Agent-based and individual-based modeling: A practical introduction.



What is it about?



B. Analyzing simulated data







A. Producing simulated data	Defining parameter combinations to run the simulation (experimental design) Determining the number of runs per setting
B. Analyzing simulated data	Finding methods and tools to analyze the simulated data Choosing relevant perspectives on data (level of detail, course of runs, avg,)
C. Communicating results	Creating an condensed overview of relevant results Using output templates and graphical representations



A. Producing simulated data	Complexity
	Focus on the research objective

B. Analyzing simulated data

Stochasticity

Non-linearities

C. Communicating results

Presentation of complex results



Focus of this talk on design of simulation experiments

A. Producing simulated data Research objective Classification of Variables Factors and Output measures Experimental design Error variance analysis B. Analyzing simulated data Effect analysis C. Communicating results Effect matrix



Step (1) Objective of the Simulation Experiment





First association with simulation models: Prediction as the objective



Source: UrbanSim Model - Modeling Land Cover Change In Central Puget Sound: The LCCM Model (urbaneco.washington.edu)- Pudget Sound, US-State: Washington

Objective: Analyzing the fitness landscape of simulation outputs

Population size, N = 2,304 Mutation rate, μ = 0.05 per trait

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Source: http://en.wikipedia.org/wiki/Fitness_landscape

What are the forces?

How are the effects of factors?

How do they interact?

Given the research question, the objective of the simulation experiment needs to be formulated to produce adequate data

- A simulation can be used for **many different issues**, for example for the characterization or optimization of models.
- The research question can only be answered if the simulation experiment produces adequate data.
- Two major objectives are typically stressed (Law 2007):
 - 1. Relative comparison of alternative simulation configurations, e.g. <u>identifying</u> <u>important factors and their effects on the response</u>.
 - 2. Performance assessment of different simulation configurations, e.g. <u>finding the optimal parameter settings</u>.

Step (2) Classification of Variables

What are the relevant parameters to answer the research question?

Parameters	- 0	٦	1	Parameters		
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Simulation Parameters		^		1_Ind	_RelAdvantag	e: 5
.% Consumertype2:	0,5			1_1	Ind_SocialValue	e: 5
.% EA:	10			1_	_Ind_Trialabilit	y: 5
.% EA Consumertype1:	0,5			2_Ind_Ad	optionIntentio	n: 5
.% EA Consumertype2:	0,5			2_In	d_Compatibilit	y: 5
.Network Type:	5			2_Ind_C	ConditionalValue	e: 5
.Number of Consumers:	100			2_	Ind_EaseofUs	e: 5
.SmallWorld Beta:	0,2			2_Ind_	EmotionalValue	e: 5
.SmallWorld Degree:	4			2_Ind_	_EpistemicValue	e: 5
1 Ind AdoptionIntention:	5			2_Ind_F	FunctionalValue	e: 5
1 Ind Compatibility:	5			2_Inc	d_Observabilit	y: 5
1 Ind ConditionalValue:	5			2_Ind	_RelAdvantage	e: 5
1 Ind EaseofUse:	5			2_1	Ind_SocialValue	e: 5
1 Ind EmotionalValue:	5			2	_Ind_Trialabilit	y: 5
1 Ind EpistemicValue:	5			Aggre	gate Indicator	s:
1 Ind FunctionalValue:	5			Cre	ate HTML Tool	s:
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The classification of model variables allows for an overview of the different types of variables based on their roles with respect to the model and its analysis

- The set of variables has to be divided into
 - the ones that are important for the given research question and
 - the ones that are not important but could affect the model behavior as well.
- Above, the variables measuring simulation performance have to be identified to be able to evaluate the model behavior.

Basic aspects of the research question can be easily communicated using the table of variables

- Based on this table one can easily read
 - which relationships are in the focus of research and
 - major questions under investigations in a standardized and condensed way
- Advantageous in an interdisciplinary context, where the relationships of interest are expressed in the "universal language" of variables and their relationships.
- Using variables might make the simulation experiment more accessible, particularly for non-experts.

Classification of Variables									
Independent variables	Control variables	Depend	lent variables						
(1) Learning algorithm	 (2) Length of equilibrium (3) Strategy set (4) Real productivity (5) Report of opponent (6) Number of ticks 	(7) Quality,(8) Speed,(9) Stability	of learning truthful reporting						

Preparation of the simulation experiment by defining

- *factors* (independent variables and control variables)
- <u>response variables</u> (dependent variables)

Transformation of variables into factors and response variables

- For the simulation experiment, quantitative or qualitative factor level value ranges, and discrete or continuous response variables have to be established.
- Potential <u>control variables</u> can be included as additional factors to understand their effects as well.
- Check of <u>factors with parameters in the program code</u> (main class parameters) assures a comprehensive list of influencing factors.

Simulation parameter (main class)	DOE		Other parameters
double lamda	\checkmark	Factor	
double T	\checkmark	Response Variable	
double T_i	-		Support parameter to calculate T (per i)
double T_max	-		Support parameter to calculate T (basis)
double[] strategies	\checkmark	Control Variable	
double pi	-		Simulation output (report)
()			

Important complication: Complex factors may have many different configurations in their substructure.

- Some factors are **complex**, having a substructure that determines their qualitative or quantitative value
- Different configurations may cause varying responses
- To make the effects of complex factors comparable, a **benchmark level for each factor level** has to be established

"Cascaded DOE" as solution

Cascaded DOE allows to identify appropriate configurations of complex factors.

In the cascaded concept we distinguish **two different DOE-Types**:

- The Top-Level-DOE is to analyze the overall research question, containing complex variables as factors
- The subordinated DOEs aim at optimal factor configurations on the level of the substructure of the complex factor

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Optimized learning algorithms performance for treatment comparison

Cascaded DOE allows to identify appropriate configurations of complex factors

Table of Factors - Top	-Level DOE, Resea	rch Question "C	omplexity of	Groves Mecha	nism"			
Factors	Factor Level Ranges			Responses				
Learning Algorithms	Zero Intelligence Reinforcement L Experience Weig	Zero Intelligence R - Reinforcement Learning T - Experience Weighted Attraction E -		Quality of learning peed truthful reporting tability				
ticks	Ν							
Out DOE Zees Intellie								
Sub-DOE Zero Intellig	Sub-Factor Level Ranges	Re	esponses					
ticks	N	R - Quality T - Speed E - Stability	of le truthful r	arning eporting				
	Sub-DOE Rein	forcement Lean	ning			_		
	Sub-Factor	s Sub- Level	-Factor Resp I Ranges		esponses			
	φ ₁ ticks	€ [0,1] N		R - Quality T - Speed E - Stability	of learning truthful reporting			
			Sub-	DOE Experienc	e Weighted Attracti	on		
			s	ub-Factors	Sub-Factor Level Ranges		Re	sponses
			ρ σ φ ₂		€ [0,1] € [0,1] € [0,1]	R T E	- Quality - Speed - Stability	of learning truthful reporting
			ticks		N N			

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Step (4) Select appropriate factorial design

Strategies		
<u>Buest-gess</u> approach	 (1) Arbitrary combination of factors (2) Outcome (3) Switching one (or two) factor levels (depending on the outcome). 	
<u>One-factor-at-a-</u> time approach	 Baseline (starting point) Varying each factor over its range Result: Effects on response value for each factor, while other factors are fixed. 	
<u>Factorial</u> experiment	Factors are varied together.	interaction

Task: To define points in the surface by which we may learn about the nature of the model.

Factorial design can deal efficiently with a large number of factors and factor level ranges

- Factorial design assures a systematic analysis of factor level combinations, so that valid and objective results are produced and interactions between factors are identified.
- The choice for the right factorial design depends on the number of factors, the factor level ranges, and the objective of the simulation experiment.

For a 2^k -factorial design only two factor levels per factor are defined. Typically one high and one low value per factor

2^k factorial Design:
k number of factors
with 2 factor levels each.
Here: k=5

Factors	Factor Level Range	Factor Levels	Respresentation
ρ	€ [0,1]	{0.15, 0.85}	{-, +}
σ	€ [0,1]	{0.15, 0.85}	{-, +}
φ ₂	€ [0,1]	{0.15, 0.85}	{-, +}
λ	€ [0,1]	{0.15, 0.85}	{-, +}
ticks	N	{1000, 5000}	{-, +}

For a 2^k-factorial design only two factor levels per factor are defined. Typically one high and one low value per factor.

2k Design		Factor Lovala	Beenreeentetion
2k Design Factors	Factor Level Range	Factor Levels	Respresentation
2k Design Factors ρ	Factor Level Range € [0,1] € [0,1]	Factor Levels {0.15, 0.85} {0.15, 0.85}	Respresentation {-, +}
2k Design Factors ρ σ	Factor Level Range € [0,1] € [0,1] € [0,1]	Factor Levels {0.15, 0.85} {0.15, 0.85} {0.15, 0.85} {0.15, 0.85}	Respresentation {-, +} {-, +} {-, +}
2k Design Factors ρ σ φ ₂ λ	Factor Level Range € [0,1] € [0,1] € [0,1] € [0,1] € [0,1]	Factor Levels {0.15, 0.85} {0.15, 0.85} {0.15, 0.85} {0.15, 0.85} {0.15, 0.85}	Respresentation {-, +} {-, +} {-, +} {-, +} {-, +}

This leads to $2^5 = 32$ design points in the design matrix to be run as simulation settings within the simulation experiment.

Based on the recorded (average) resonse values in the design matrix, the factor effects are calculated.

	Factors								
DP	ticks	ρ	σ	φ2	λ				
1									
2	-		-	-	+				
3	-	-	-	+	-				
4	-		-	+	+				
5	-	-	+	-	-				
6	-	-	+	-	+				
7	-	-	+	+	-				
8	-	-	+	+	+				
9	-	+	-	-	-				
10	-	+	-	-	+				
11	-	+	-	+	-				
12	-	+	-	+	+				
13	-	+	+	-	-				
14	-	+	+	-	+				
15	-	+	+	+	-				
16	-	+	+	+	+				
17	+	-	-	-	-				
18	+	-	-	-	+				
19	+	-	-	+	-				
20	+	-	-	+	+				
21	+	-	+	-	-				
22	+	-	+	-	+				
23	+	-	+	+	-				
24	+	-	+	+	+				
25	+	+	-	-	-				
26	+	+	-	-	+				
27	+	+	-	+	-				
28	+	+	-	+	+				
29	+	+	+	-	-				
30	+	+	+	-	+				
31	+	+	+	+	-				
32	+	+	+	+	+				

Step (5) Estimation of experimental error variance

Stochastic elements in simulation models cause a variance in the simulation output.

For an initial estimation of the number of simulation runs required per simulation setting, the size of the experimental error needs to be analyzed

- Simulation models often contain **stochastic elements**, resulting in **non-deterministic simulation responses**.
- The fluctuation would **distort the analysis of outcome differences** between simulation settings.
- In order to obtain meaningful results, the mean and variance over several simulation runs per setting must be analyzed (Gilbert 2008).
- As a first approximation of the needed number of runs per setting, the **experimental error analysis** is performed.

Toy Model: Error variance analysis for normal distributed random numbers $\in [0,1]$

Error Variance Analysis

Task:Finding N with **stable variance** and the **respresentative mean**, Knowing more about the **error (here: deviation from 0.5)**

Error Variance Matrix

Increasing the number of repetitions typically stabilizes the variability of the response to a point when c_v with increasing N does not change any more

Error Variance	Matrix											
				Number of Runs								
Design Point		dep. Variables	10	100	500	1000	5000	10000	20000	40000	60000	80000
	R	MEAN VARIANCECOEFF	0.70 0.02									
1.VA	т	MEAN VARIANCECOEFF	361.90 0.28	524.01 0.34	500.26 0.38	498.88 0.37	502.03 0.38	503.25 0.37	503.94 0.37	502.71 0.37	503.11 0.37	502.25 0.37
	E	MEAN VARIANCECOEFF	0.01 0.67	0.01 0.93	0.01 0.93	0.01 0.94	0.01 0.95	0.01 0.95	0.01 0.95	0.01 0.95	0.01 0.95	0.01 0.95
							Numb	er of Runs				
Design Point		dep. Variables	10	100	500	1000	5000	10000	20000	40000	60000	80000
	R	MEAN VARIANCECOEFF	0.66 0.02									
2. VA	т	MEAN VARIANCECOEFF	400.30 0.33	522.90 0.37	525.89 0.37	517.81 0.38	513.88 0.38	516.75 0.37	517.92 0.37	515.27 0.37	515.70 0.37	518.83 0.37
	E	MEAN VARIANCECOEFF	0.01 0.73	0.01 0.94	0.01 1.09	0.01 1.03	0.01 1.01	0.01 1.01	0.01 1.01	0.01 1.01	0.01 1.01	0.01 1.02
							Numb	er of Runs	_			
Design Point		dep. Variables	10	100	500	1000	5000	10000	20000	40000	60000	80000
	R	MEAN VARIANCECOEFF	0.66 0.03	0.67 0.02	0.66 0.03	0.67 0.03	0.67 0.03	0.67 0.03	0.70 0.02	0.67 0.03	0.66 0.03	0.66 0.03
3.VA	Т	MEAN VARIANCECOEFF	514.70 0.25	513.45 0.32	488.99 0.40	515.62 0.37	515.46 0.37	513.27 0.37	503.94 0.37	515.90 0.37	516.46 0.37	515.71 0.37
	E	MEAN VARIANCECOEFF	0.01 1.00	0.01 0.96	0.01 0.91	0.01 0.97	0.01 1.01	0.01 1.02	0.01 0.96	0.01 1.01	0.01 1.01	0.01 1.01

Limitations of the error variance analysis

- The experimental error needs to be interpreted with respect to the respective model.
- General criteria might not be applicable to the given model, e.g. the variability of the response variables does not stabilize over an affordable number of runs.
- Definition of number of runs required is a tradeoff between stability and costs. As in empirical research, more points of observations bring accuracy, but produce cost.
- Error variance analysis should result in **a first impression of the error variance** and in the ability to approximate the required number of runs per setting for the simulation experiment.
- It should provide a tool for determining the number of runs and thus for communication and transparency of the criteria.

Filling the *design point matrix* with response variable values

- The simulation experiment is performed to produce the simulation data.
- The factor level combinations are given from the factorial design (4.).
- For every design point, N simulation runs are performed, as given from the analysis of error variance (5.).
- The response values are recorded as average values over N runs.

Design	n matrix S	Sub-DOE	EWA]
			Factors				Response		
DP	ticks	ρ	σ	φ2	λ	R	Т	Ε	
1	-	-	-	-	-	0.705	456.487	0.012	
2	-	-	-	-	+	0.731	181.767	0.052	
3	-	-	-	+	-	0.734	364.125	0.022	
4	-	-	-	+	+	0.783	207.305	0.104	
5	-	-	+	-	-	0.705	457.304	0.012	
6	-	-	+	-	+	0.731	181.033	0.052	
7	-	-	+	+	-	0.734	367.212	0.022	Basis
8	-	-	+	+	+	0.784	206.150	0.105	for
9	-	+	-	-	-	0.699	512.463	0.009	
10	-	+	-	-	+	0.706	461.628	0.012	data
11	-	+	-	+	-	0.705	484.552	0.011	
12	-	+	-	+	+	0.735	362.173	0.022	analysis
13	-	+	+	-	-	0.699	509.315	0.009	/
14	-	+	+	-	+	0.705	461.081	0.012	
15	-	+	+	+	-	0.705	484.614	0.010	
16	-	+	+	+	+	0.735	361.748	0.022	
17	+	-	-	-	-	0.705	462.672	0.018	
18	+	-	-	-	+	0.732	182.305	0.053	
19	+	-	-	+	-	0.737	368.752	0.025	
20	+	-	-	+	+	0.800	222.256	0.109	
21	+	-	+	-	-	0.705	458.574	0.018	
22	+	-	+	-	+	0.732	180.379	0.053	
23	+	-	+	+	-	0.737	367.273	0.025	
24	+	-	+	+	+	0.799	226.051	0.109	
25	+	+	-	-	-	0.699	512.191	0.016	
26	+	+	-	-	+	0.705	459.364	0.018	
27	+	+	-	+	-	0.705	483.745	0.017	
28	+	+	-	+	+	0.737	361.640	0.025	
29	+	+	+	-	-	0.699	517.674	0.016	
30	+	+	+	-	+	0.706	459.273	0.018	
31	+	+	+	+	-	0.705	490.982	0.017	
32	+	+	+	+	+	0.737	358.334	0.025	

Step (7) Analyzing effects

Within the effect analysis we determine factor effects, interaction effects and control variables as major results

- Basis for the effect analysis is the design matrix, as defined by the **factorial design**.
- Within the effect analysis, we determine the simulation results by
 - the effect of every factor on all response values in strength and direction,
 - check for possible interaction effects between factors, and
 - fix potential control variables, if they have no or a nominal effect on the response (result for sensitivity analysis)

Basis for analysis: Design point matrix

Design matrix Sub-DOE EWA								
			Factors				Responses	;
DP	ticks	ρ	σ	φ2	λ	R	Т	E
1	-	-	-	-	-	0.705	456.487	0.012
2	-	-	-	-	+	0.731	181.767	0.052
3	-	-	-	+	-	0.734	364.125	0.022
4	-	-	-	+	+	0.783	207.305	0.104
5	-	-	+	-	-	0.705	457.304	0.012
6	-	-	+	-	+	0.731	181.033	0.052
7	-	-	+	+	-	0.734	367.212	0.022
8	-	-	+	+	+	0.784	206.150	0.105
9	-	+	-	-	-	0.699	512.463	0.009
10	-	+	-	-	+	0.706	461.628	0.012
11	-	+	-	+	-	0.705	484.552	0.011
12	-	+	-	+	+	0.735	362.173	0.022
13	-	+	+	-	-	0.699	509.315	0.009
14	-	+	+	-	+	0.705	461.081	0.012
15	-	+	+	+	-	0.705	484.614	0.010
16	-	+	+	+	+	0.735	361.748	0.022
17	+	-	-	-	-	0.705	462.672	0.018
18	+	-	-	-	+	0.732	182.305	0.053
19	+	-	-	+	-	0.737	368.752	0.025
20	+	-	-	+	+	0.800	222.256	0.109
21	+	-	+	-	-	0.705	458.574	0.018
22	+	-	+	-	+	0.732	180.379	0.053
23	+	-	+	+	-	0.737	367.273	0.025
24	+	-	+	+	+	0.799	226.051	0.109
25	+	+	-	-	-	0.699	512.191	0.016
26	+	+	-	-	+	0.705	459.364	0.018
27	+	+	-	+	-	0.705	483.745	0.017
28	+	+	-	+	+	0.737	361.640	0.025
29	+	+	+	-	-	0.699	517.674	0.016
30	+	+	+	-	+	0.706	459.273	0.018
31	+	+	+	+	-	0.705	490.982	0.017
32	+	+	+	+	+	0.737	358.334	0.025

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Calculation of Effect Sizes

Interaction Effect Size

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The effect matrix allows for a condensed representation of simulation results in a standardized way

To structure the results we fill an **effect matrix for every response value**, containing the factor effects of each factor and all interaction effects between factor pairs.

Effect Matrix					
response variable <i>R</i> _i	factor x ₁	factor x ₂	factor x ₃	factor x ₄	factor x ₅
factor x ₁	main effect X 1	interaction effect (x 1, x 2)	interaction effect (X 1,X 3)	interaction effect (x 1, x 4)	interaction effect (x ₁ ,x ₅)
factor x ₂		main effect x ₂	interaction effect (x 2, x 3)	interaction effect (x ₂ , x ₄)	interaction effect (x ₂ , x ₅)
factor x ₃			main effect X 3	interaction effect (x ₃ ,x ₄)	interaction effect (x ₃ ,x ₅)
factor x ₄				main effect x₄	interaction effect (x ₄ ,x ₅)
factor \mathbf{x}_5					main effect x 5

	resources	minValue	prodScale	capacities	reductProd	discount
resources	21.5	9.93	8.65	3.88	-2.78	14.35
	(21.53, 21.47)					
minValue	-	10.83	0.03	-0.01	0.01	7.23
		(10.83, 10.83)				
prodScale	-	-	9.43	0.03	-0.34	6.32
			(9.36, 9.51)			
capacities	-	-	-	4.23	2.52	2.84
				(5.38, 3.08)		
reductProd	-	-	-	-	-3.05	-2.03
					(-3.24, -2.86)	
discount	-	-	-	-	-	15.65
						(15.6, 15.69)

Table 7.5.: Effect matrix - LAMDA I (mean differences)

Table 7.6.: Effect matrix – LAMDA I (standardized β from regression analysis, $R^2 = 0.865$, adjusted $R^2 = 0.865$, Signif. codes: p<0.001='***', p<0.01='**', p<0.05='*', N=729.000)

	resources	minValue	prodScale	capacities	reductProd	discount
resources	0.558***	-0.211***	0.183***	0.083***	-0.059***	0.304***
	(p=0.000)	(p=0.000)	(p=0.000)	(p=0.000)	(p=0.000)	(p=0.000)
minValue	-	0.281***	0.001	0.000	0.000	0.153***
		(p=0.000)	(p=0.137)	(p=0.816)	(p=0.483)	(p=0.000)
prodScale	-	-	0.245***	0.001*	-0.007***	0.134***
			(p=0.000)	(p=0.034)	(p=0.000)	(p=0.000)
capacities	-	-	-	0.111***	0.054***	0.061***
				(p=0.000)	(p=0.000)	(p=0.000)
reductProd	-	-	-	-	-0.079***	-0.043***
					(p=0.000)	(p=0.000)
discount	-	-	-	-	-	0.406***
						(p=0.000)

Mean difference vs. standardized beta (regression analysis)

- Often, simulation models are **too complex** for a full factorial design.
- DOE provides techniques to **reduce** the simulation analysis **complexity** (see *fractional factorial design*).
- Still, other techniques above systematic DOE might be used to reduce the model complexity. As there are:
 - switching certain mechanisms on/off,
 - simplifying scenarios,
 - making environment constant/homogeneous,
 - using zero intelligence agents.
- These techniques are proposed to be defined at the beginning of the analysis process and can be used **as benchmark** for increasing model complexity.
- Iterative analyses based on the DOE process can be conducted for these scenarios.

The issues presented are addressed in a systematic procedure to apply DOE principles for simulation experiments.

What is it about?

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Lorscheid, Iris, Bernd-Oliver Heine und Matthias Meyer. (2012) Opening the 'black box' of simulations: increased transparency and effective communication through the systematic design of experiments. *Computational and Mathematical Organization Theory*. 18(1):22-62 -- DOI: 10.1007/s10588-011-9097-3

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