Global Sensitivity Analysis: Elementary Effects Method of Morris using Sampling for Uniformity (SU) MatLab code manual

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1. Elementary Effects Sampling Package Including Sampling for Uniformity (SU)

There are two Elementary Effects (EE) packages that complement the analysis: a) *EE Sampling* - to obtain the Morris samples based on a number of methods, including Sampling for Uniformity (SU); and b) *EE Measures and Plots* - after running the model with the EE samples it post-processes the results and provides Morris statistics and plots.

Download the Matlab code, sample inputs and documentation for the packages from the links below:

- <u>EE Sampling for Matlab</u> [10kB]
- <u>EE Measures and Plots for Matlab</u> [10kB]
- This documentation in PDF (1.4 MB)

Please click on the tabs below to see the documentation for each of the packages.

- <u>EE Sampling</u> |
- <u>EE Measures and Plots</u>

Description

EE_Sampler_Mapper Package is a set of MATLAB functions that generates input factor samples for the method of Elementary Effects or Morris method (Morris, 1991). The main function to run is 'Fac_Sampler.m' (or its simplified command line form sampler.m). It generates input factor samples in a unit hyperspace and then transforms them according to the specified input probability distributions. Currently this code gives five options for sampling strategy: (a) the method of Optimized Trajectories [OT] (Campolongo et al. 2007); (b) the Modified Optimized Trajectories [MOT] (Ruano et al., 2012); (c) Sampling for Uniformity [SU] (Khare et al., 2015); and (d) Enhanced Sampling for Uniformity [eSU] (Chitale et al., 2017); and e) RadialeSU (Khare et al.) (in preparation).

Program Usage & Outputs

Syntax

Fac_Sampler('facfile', 'SS', OvrSamSiz, NumLev, NumTraj, 'SamFileType')

A command line shell (sampler.m) is provided for those interested in compiling the program for use in mixed environments (i.e. unix scripts and others). The program can be compiled in the matlab environment with 'mcc m sampler.m'. This will produce a command line executable that can be run outside Mtatlab, or in another machine command line environment provided that the same runtime library version as the compiler is installed in the client machine (see Matlab Compiler Runtime download and instructions <u>here</u>). An example of use for this tool (inside and outside Matlab) would be:

sampler 'try.fac' 'eSU' 1 8 16 'Text'

Inputs:

(1) facfile. This is an ASCII '.fac' file that that follows the format (and can be generated) from SimLab v2.2. For exact file formatting and distribution characteristics please refer SimLab v2.2 manual App. C (<u>available here</u>). The file contains the following information:

(a) number of input factors (NumFact)

(b) default distribution truncation values

(c) distribution type and distribution characteristics for each input factor.

(2) SS: Sampling Strategy. Currently we provide five options:

(a) 'OT' - Campolongo et al. (2007) - Method of Optimized Trajectories

(b) 'MOT' - Ruano et al. (2012) - Method of Modified Optimized Trajectories

(c) 'SU' - Khare et al. (2015) - Sampling for Uniformity

(d) 'eSU' - Chitale et al. (2017) – Enhanced Sampling for Uniformity

(e) 'RadialeSU' - Khare et al. (in preparation) – Radial eSU

(3) OvrSamSize: Oversampling Size.

For OT and MOT the recommended oversampling size is 500-1000. For SU recommended oversampling size is 300. For eSU oversampling is not necessary i.e. we recommend OvrSamSize = 1. The current version of this EE_SamplerMapper tool interactively guides user to choose appropriate Oversampling size based on literature recommendations.

(4) NumLev: Number of input factor levels

In EE literature various values for number of levels have been suggested. However, the standard practice is to use even number of levels usually 4, 6 or 8. For SU/eSU and RadialeSU user can choose from NumLev = {4,6,8,10,12,14,16}. If user specifies NumLev that does not belong to this set, then it will be set to 4 by default.

(5) NumTraj: Number of trajectories to be generated

In EE literature recommended value for number of trajectories vary from

as little as 2 to as large as 100. However, a number of studies have reported that 10-20 trajectories are sufficient. For eSU the number of trajectories should be multiple of the number of levels to get better results. The current version of this EE_SamplerMapper tool interactively guides user to change/select number of trajectories whenever necessary.

(6) SamFileType: Sample File Format. Currently we provide two options:

- (a) 'Excel'
- (b) 'Text' (comma separated file with .sam extension)

Outputs:

(1) Factor_Sample : Input factor sample [ncol,nrows], where ncol = NumFact and nrows = NumTraj*(NumFact+1). Each column corresponds to a input factor

(2) *_FacSample.xlsx or *_FacSample.sam:

If user sets SamFileType = 'Excel' then Factor samples are written to an excel file '*_FacSample.xlsx', where * i.e. first part of the file name is same as the first part of the '.fac' file. (e.g. Factor sample for the input file 'Example.fac' will be saved in 'Example_FacSample.xlsx'). If user sets SamFileType = 'Text' then Factor samples are written to a text file '*_FacSample.sam', where * (i.e. first part of the file name) is the same as the first part of the '.fac' file. In both types of files each column corresponds to a factor. Factor name is specified on the first row

(3) *_FacSamChar.txt: Characteristics used for generating the sample are written to a text file '*_FacSamChar.txt, where * i.e. first part of the file name is same as the first part of the '.fac' file. (e.g. FacSamChar file for the input file 'Example.fac' will be saved as 'Example_FacSamChar.txt'). Details of

*_FacSamChar.txt file are as follows

First Line: Sampling Strategy – OT, MOT, SU, eSU or RadialeSU

Second Line: Oversampling Size

Third Line: Number of levels

Fourth Line: Number of trajectories

Fifth Line: Number of factors

Folder Structure:

There are 6 Matlab functions (i.e. m files) and five folders (Campolongo, Ruano, Khare, and Enhanced_Khare, Radial_Khare) included in this package (EE_Sampler_Mapper). Generated factor/input factor sample file *_FacSample.xlsx' or '*_FacSample.sam' and '*_FacSamChar.txt' will be stored in the folder same as 'Fac_sampler.m'.

Input Factor Probability Distributions for facfile:

Currently following parameter distributions can be generated using this package. For the details about distribution characteristics please refer SimLab v2.2 user manual App A (available <u>here</u>).

- (1) 'Uniform'
- (2) 'LogUniform'
- (3) 'Normal'
- (4) 'LogNormal'
- (5) Discrete (for categorical factors)

'Nominal' - uniform discrete for nominal factors

'NUDiscrete' - non-uniform discrete for nominal and ordinal factors

'UDiscrete' – uniform discrete for ordinal factors.

(6) 'Constant'
(7) 'Triangular'
(8) 'Weibull'
(9) 'Beta'
(10) 'Gamma'
(11) 'Exponentia'l
(12) 'Log10Uniform'

Note on Discrete Distributions. To make EE_SamplerMapper tool more flexible in its usage. we replaced the original simlab 'Discrete' distribution by the three types presented above ('Nominal', 'NUDiscrete', and 'UDiscrete')

Two types of discrete factors are considered. *Nominal* factors refer to categories where the order does not matter (i.e. all categories have the same probability). Examples of nominal factors are gender, nationality, land use categories, etc. *Ordinal* factors refer to categories where the order matters (for example, 'low', 'medium', 'high'). Both factors can be selected with uniform and non-uniform discrete distributions.

'Nominal' distribution is used for nominal factors of equal probability, i.e. discrete uniform distribution. For these factors, it is necessary to ensure that all combinations of discrete levels are considered to get reliable EE based sensitivity measures. However, this increases the number of trajectories. Current version of the EE_SamplerMapper guides users to select appropriate number of trajectories i.e. NumTraj when it encounters the presence of 'Nominal' factors. Example: If modeler is to choose from a number of sub-models to be used to simulate a particular mechanism then that 'sub-model' is a factor with nominal discrete type of factor. There is no restriction on number of discrete values/categories/options to be selected. However, larger

the number of categories larger is the number of trajectories needed.

'NUDiscrete' distribution can be currently used only for ordinal factors with non-uniform distributions. However, users must be cautious when using this option. Note that this distribution can result in one or more trajectories where one or more factors do not change values, with potentially inaccurate EE measures/ EE Screening. Accuracy of generated factor distributions depends on Number of Factor Levels used for sampling. E.g. for SU and eSU if NumLev is 4, then only three non-uniform probability configurations can be generated for NUDiscrete factors -25%, 25%, 25%, 25%, 25%, 25%.

'UDiscrete' distribution can be used for ordinal factors with the same probabilitiy, i.e. discrete uniform distributions. Like NUDiscrete distribution successful generation of sample depends on NumLev used.

The use of the three discrete distributions is restricted to SU, eSU and RadialeSU. EE_Sampler_Mapper tool prompts user to choose appropriate sampling method when these types of distributions are present. We are currently expanding our tool to improve its utility in generation one more distribution – non-uniform nominal/NUNominal distribution. Please contact the authors for additional information if this feature is needed.

Probability distribution truncation

(A) When parameter distribution/distributions have long tails (Normal, LogNormal, Weibull, Gamma, Exponential), to get accurate results/ parameter rankings consistent with variance-based SA methods (e.g. Sobol'), experience has shown that truncated distributions perform better. SimLab v2.2 truncates distributions at 12.5% and 87.5% i.e. overall 25% truncation. Though, ideal truncation may vary from model to model, we recommend 2.5% to 5% truncation from either side. (B) If user wants to use different truncations for different factors/parameters lower and upper percentiles (expressed as fractions) should be edited in the .fac' (please refer to App. C of SimLab v2.2 manualSimLab v2.2 manual App. C available here). By default SimLab v2.2 sets these values these values at 0.001 and 0.999. See Example 2 in the following sections for additional details.

Input/Output Examples

Example 1

Generate 10 trajectory samples for factor file 'Example1.fac' (see package distribution) with OT method. Use oversampling size of 500 and 6 factor levels. Save outputs in text format (Example1_FacSample.sam). Type following in the Matlab Command window making sure that you are in EE_Sampler_Mapper folder.



Output (notice new files Example1_FacSamChar.txt and Example1_FacSampler.sam on the left column)



Example 2

Generate samples for factors in 'Example2.fac' (see package distribution) using method of MOT. Generate 8 trajectories with 500 oversampling size, NumLev = 4. Save sample in excel format. Note that Example2.fac contains 'Nominal' and 'UDiscrete' type factors.Type following in Matlab command window.



Output:

Command Window	
(1) New to MATLAB? Watch this <u>Video</u> , see <u>Examples</u> , or read <u>Getting Started</u> .	
ERROR: You have 1 categorical factors with multiple (> 2) categories	
Method of OT does not handle this type of distributions	

RECOMMENDATION: Consider SU/eSU(preferred)/RadialeSU for sample generations	
Annaly successed	
Sample was not generated	
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As expected, the sample was not generated and a warning is shown

Following the warning, we now generate the samples using eSU instead of MOT. Keep all other settings the same, except OverSamSiz = 1.



In this case, due to the presence of Nominal factors, user was asked to increase number of trajectories as shown. Let's increase number of trajectories to 40.



Example 3

Generate samples for factors in 'Example3.fac' (see package distribution) using method of eSU. Generate 10 trajectories with 100 oversampling size,

NumLev = 10. Save sample in text format. Type following in Matlab command window.



Output



Lets try generating sample for Example3.fac file with eSU. Try NumLev = 12, NumTraj = 8, OvrSamSiz = 1. Below are input and output screenshots



Since NumTraj = 8 is less than NumLev = 12, NumTraj will be increased to 12 to ensure uniformity of generated sample.

Output



Example 4

Generate samples for factors in 'Example4.fac' (see package distribution) using method of RadialeSU. Generate 15 trajectories with 1 oversampling size, NumLev = 12. Save sample in text format. Type following in Matlab command window.



Since NumTraj is not multiple of NumLev, NumTraj will be increased to 24 (12x2)

Output



Program License

These Matlab (R) packages were developed by Drs. Yogesh Khare and Rafael Muñoz-Carpena. This program is distributed as Freeware/Public Domain under the terms of GNU-License. If the program is found useful, the authors ask that acknowledgment is given to its use in any resulting publication and the authors notified. The source code is available from the authors upon request.

We highly encourage using these packages for EE (Morris) sampling and sensitivity measures calculations with the eSU ('enhanced Sampling for Uniformity') method. If you use this package, kindly acknowledge our effort. Also, if you have any question in usage of this package, please contact us on the email address below.

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2. Elementary Effects Measures and Plots Package Including Sampling for Uniformity

There are two Elementary Effects (EE) packages that complement the analysis: a) *EE Sampling* - to obtain the Morris samples based on a number of methods, including Sampling for Uniformity (SU); and b) *EE Measures and Plots* - after running the model with the EE samples itpost-processes the results and provides Morris statistics and plots.

Download the Matlab code, sample inputs and documentation for the packages from the links below:

- EE Sampling for Matlab [10kB]
- EE Measures and Plots for Matlab [10kB]
- <u>This documentation in PDF</u> (2.9 MB)

Please click on the tabs below to see the documentation for each of the packages.

- EE Sampling
- EE Measures and Plots

Elementary Effects (EE) Measures and Plots Package

Description

EE_SensitivityMeasures_Package is a set of Matlab functions that calculates sensitivity measures for the method of Elementary Effects/Morris method (Morris, 1991). Function 'EE_SenMea_Calc.m' is the main function that user

needs to call from MATLAB command line. Calculated measures include modified sensitivity measures – μ^* and σ based on (Campolongo et al. 2007) and original measure μ proposed by Morris (1991).

Program Usage & Outputs

Syntax

EE_SenMea_Calc ('FacFile','Fac_Sam_File','Fac_Sam_Char','Mod_Out_File')

Inputs:

(1) FacFile: This is an ASCII input factor '.fac' file that that follows the format (and can be generated) from SimLab v2.2. For exact file formatting and distribution characteristics please refer SimLab v2.2 manual App. C (available here). Please see also the EE Sampling section for additional details.

(2) Fac_Sam_File: This is '*.xlsx' file or '*.sam' file (a comma separated text file) containing factor/parameter samples. This file is generated by Factor_Sampler_Mapper package for factor sample generation.

(3) Fac_Sam_Char: This file is generated along with '*.xlsx' file or '*.sam by Factor_Sampler_Mapper package for factor sample generation. This is a '*.txt' file which contains following information

- (a) Sampling Strategy (line 1)
- (b) Over Sampling Size (line 2)
- (c) Number of factor levels (line 3)
- (d) Number of trajectories (line 4)

(e) Number of factors (line 5)

(4) Mod_Out_File: This is a '*.xlsx' file or '*.out' file (a comma separated text file) containing model outputs arranged column-wise. Output names should be specified in the first row. Currently this code can analyze only scalar outputs. In future provisions will be made for the time series outputs.

Outputs:

(1) EE_SA_Measures.txt: Sensitivity measures based on the method of Elementary Effects/ Morris method are saved in this text file, for each model output.

(2) Plots: Two figures/subplots are produced for each model output. The first subplot is a plot of μ^* vs σ while the second one consists of μ vs σ . We additionally plot $\mu^* = \sigma$ line (dotted black line) on first sub-plot and $\mu = +/-2 \sigma/sqrt(r)$ lines (solid black line) on the second subplot. In respective sub-plots factors above the line can be considered to have dominant interaction effects. $\mu^* = \sigma$ and $\mu = +/-2 \sigma/sqrt(r)$ criteria are based on Khare et al. (in preparation) and Morris (1991) to respectively. Additionally, factors for which $\mu^* = abs(\mu)$ holds true i.e. perfectly monotonic effects are indicated by solid circles. Plots are automatically saved as PDF files.

Folder Structure:

This package consists of 6 Matlab functions (i.e. m files namely (a) EE_SenMea_Calc, (b) EE_Plots, (d) Morris_Measures, (e) Morris_Measure_Radial, (f) EE_Rad_Traj) and (g) ReadFacDist saved in folder 'EE_SensitivityMeasures'. Output files – 'EE_SA_Measures.txt' and plots (PDFs) will be saved in the package folder.

For the demonstration purpose we have provided input files required for

each of the following four examples with this package. Please note that if users decide to generate their own samples from EE_Sampler Mapper_Package then they should also recalculate example model outputs. In such case EE measures would differ from the ones presented below.

Examples of syntax:

(a) If both sample and model output files are excel (.xlsx) files.

EE_SenMea_Calc ('Example_FacFile.fac','Example_Sample.xlsx','Example_SampleChar.txt','Exa mple_Output.xlsx')

(b) If sample file is *.sam and model output file is *.out

EE_SenMea_Calc ('Example_FacFile.fac','Example_Sample.sam','Example_SampleChar.txt','Exa mple_Output.out')

(c) If sample file is *.sam and model output file is *.xlsx

EE_SenMea_Calc ('Example_FacFile.fac','Example_Sample.sam','Example_SampleChar.txt','Exa mple_Output.xlsx')

(d) If sample file is *.xlsx and model output file is *.out

EE_SenMea_Calc ('Example_FacFile.fac','Example_Sample.xlsx','Example_SampleChar.txt','Exa mple_Output.out')

Input/Output Example

Example 1

This is based on Example1 sample generated in the EE_SamplerMapper package documentation.

Model output:

 $y = \prod_{i=1}^{k} P_i$

Model outputs results were saved in 'Example1_Mod_Out.xlsx' file. To calculate EE measures, first copy previously generated -'Example1_FacSample.sam' and 'Example1_FacSamChar.txt' files to EE_SensitivityMeasures Package. Then type following in Matlab command window (make sure that EE_SensitivityMeasures Package is the active Matlab folder):



Package will produce following figure, which is automatically saved as a PDF file. EE sensitivity indices (Mu*, mu and sigma) are also written to 'Example1_EE_Measures.txt'. Both files are saved in EE_SensitivityMeasures package.



Note: FacSample for this example was generated using method of OT. Since, P1, P2 and P3 had same factor distribution it is expected for them to have identical sensitivity measures. However, these results indicate that is not the case.

Example 2

This is based on Example1 sample generated in the EE_SamplerMapper package documentation.

Model Output2:

$$y1 = (\sum_{1}^{7} Pi) \left(\frac{P9}{10} + \frac{P9}{1000} + \frac{P10}{100000} \right) + \prod_{11}^{16} Pi$$

 $y2 = P1^{2} + (P2 * P3) + \exp(P4 + P5 + P6 + P7)$

Model outputs results were saved in 'Example2_Mod_Out.xlsx' file. To calculate EE measures, first copy previously generated -'Example2_FacSample.xlsx' and 'Example2_FacSamChar.txt' files to EE_SensitivityMeasures Package. Then type following in Matlab command window (make sure that EE_SensitivityMeasures Package is the active Matlab folder):



Output:



) in a	mphil. I.I., M	Name of C						
	10							
	Techane	100 T	mu nigna					
	11	3.3994e=12	3.3034e+02	3.3446+12				
	80	3.3994e+02	3.3094e+02	3.3440e+02				
	F3	3.3994e+02	3.3094e+02	3.304/0+02				
	14	6.6383e+00	4.4382+01	4.0723e+01				
	15	6.43838-00	6.42828+01	6.07234401				
	216	6,43038-05	4.4002w=01	4.07234+01				
	97	6.4363e=05	4.4382x+03	4.01234+01				
	11	3.2143e+02	2.5349e+02	4.983Ge+02				
	2.2	2.3803e+02	1.3737e+03	3.1448+102				
	800	1.3146+02	7.2004e+00	3.8238++02				
	P21	4.4743+11	4,47434401	4.54538+03				
14	122	4.4175e+01	4,41754-00	4.52044-03				
	12.0	4.7942e+01	4,79424+05	5.9669e+13				
	154	5.3333e+01	5.5313e+01	7.3428e+03				
	1911	3.3850e+01	5.5950e+05	7.8228++03				
	104	3.4830e+01	5.4850e+00	6.0023++03				
	¥2							
	factures	10 m m	mu nigna					
	11	1,4047e+00	7.9934e-14	1.43204+01				
	12	9.2900e+00	0.0000e+00	1.1797e+01				
24	12	9.2900e+00	-8.8000e-38	3.37978+03				
	14	9.3003e+00	9.3000m+00	4.52274+00				
	15	8,98566+00	0.90568+00	5,44224+00				
	14	9,60736-00	9.4079e+00	4.76024+00				
	6.3	3,0329e+05	1.01294+01	7,79084=00				
	210	0.0000e+00	0.0000e+00	0.0000e+00				
	1.0	0.0000e+00	0.0000e+00	0.0000e+00				
	100	0.0000+00	0.0000+00	0.0000+00				
	P11	0.0000+00	0.00004+00	0.0000+00				
	122	0.00004+00	0.00004-00	0.0000e+00				
14	12.2	0.0000e+00	0.0000e+00	0.0000e+00				
	154	0.0000e+00	0.0000e+00	0.0000e+00				
	121	0.0000e+00	0.0000e+00	0.0000e+00				
	124	0.0000+00	0.0000e+00	0.0000e+00				
100	the file		serger: LMP lines	10 IA 1 G	P. 1 . Sec. 1919	Linux (EF)	10.4	86

Note: The sample for this example was generated with the eSU method. For the second output (y2), it was expected that (1) P8 to P16 will have zero sensitivity indices, (2) P2 and P3 should have identical sensitivity indices due to their distributions and nature of output function, (3) P4 to P7 should have identical indices, and (4) P1, P2 and P3 would be non-monotonic. From the calculated indices three of these four things were found to be true. Though sensitivity measures for P4 to P7 were not identical they were relatively close.

Example 3

This is based on Example 3 sample generated in the *EE Sampling* package documentation (please see details following the link on top of this page).

Model Output :

 $y = \sum_{i=1}^{n} P_i$

Model outputs results were saved in 'Example3_Mod_Out.out' file. To calculate EE measures, first copy previously generated -'Example3_FacSample.sam' and 'Example3_FacSamChar.txt' files to EE_SensitivityMeasures Package. Then type following in Matlab command window (make sure that EE_SensitivityMeasures Package is the active Matlab folder):



Package will produce following figure, which is automatically saved as a

PDF file. EE sensitivity indices (Mu*, mu and sigma) are also written to 'Example3_EE_Measures.txt'. Both files are saved in EE_SensitivityMeasures package.



Example 4

This is based on Example4 sample generated in the EE_SamplerMapper package documentation based on 'RadialeSU' method.

Model Outputs:

$$Y1 = \sum_{i=1}^{10} \frac{1}{1 + P_i}$$

$$Y2 = (\sum_{1}^{3} Pi)(\prod_{4}^{7} Pi)(\sum_{8}^{10} \frac{Pi}{10^{i-6}})$$

Model outputs results were saved in 'Example4_Mod_Out.xlsx' file. To calculate EE measures, first copy previously generated - 'Example4_FacSample.sam' and 'Example4_FacSamChar.txt' files to EE_SensitivityMeasures Package. Then type following in Matlab command window (make sure that EE_SensitivityMeasures Package is the active Matlab folder):



With output:



ample4	UEE_M	easures.bd 🔛		
¥1				
fac	cname	ma*	mu sigma	
P1		5.8517e+00	-2.7067e+00	7.9975e+00
P2		4.0508e+00	1.5008e+00	4.7585e+00
£3		2.7614e+00	2.7614e+00	4.7671e+00
24		4.7619e-01	-4.7619e-01	1.0583e-01
₽5		4.7619e-01	-4.7619e-01	1.0583e-01
26		4.7619e-01	-4.7619e-01	1.0583e-01
27		4.7619e-01	-4.7619e-01	1.0583e-01
198		9.9491e-01	-9.9491e-01	2.9426e-01
129		1.0008e+00	-1.0008e+00	5.1883e-01
P10	0	9.5023e-01	-9.5023e-01	6.4551e-01
¥2				
fac	cname	ma*	mu sigma	
P1		3.0443e+03	3.0443e+03	1.4315e+04
P2		6.3487e+03	6.3487e+03	2.8646e+04
P3		3.0617e+04	3.0617e+04	1.4313e+05
P4		1.1863e+04	9.2253e+03	5.2214e+04
25		9.1719e+03	7.7144e+03	4.1546e+04
26		8.5132e+03	6.8556e+03	3.7872e+04
27		1.1232e+04	7.7459e+03	4.6629e+04
50		5.1112e+02	2.9296e+02	1.9121e+03
29		1.6806e+03	-1.6522e+03	5.7349e+03
P10	5	2.2695e+04	5.3738e+03	8.2338e+04

Program License

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We highly encourage using these packages for EE (Morris) sampling and sensitivity measures calculations with the eSU ('enhanced Sampling for Uniformity') method. If you use this package, kindly acknowledge our effort. Also, if you have any question in usage of this package, please contact us on the email address below.

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APPENDIX A: PROBABILITY DISTRIBUTION FUNCTIONS FOR INPUT FACTORS USED © SIMLAB V2.2.1, EU JCR ISPRA

Normal distribution

The density function of the Normal distribution has the following expression:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[\frac{-1}{2}\left[\frac{x-\mu}{\sigma}\right]^2\right]$$

for x in $(-\infty, \infty)$.



Figure 89 Normal distribution panel

• Mean value (μ), with μ in (- ∞ , ∞); the default value is $\mu = 0e+000$.

2 Standard deviation value (σ), with $\sigma > 0$; the default value is $\sigma = 1e+000$.

3 Truncation value; the default value is in [0.001, 0.999].

There is the possibility to see the density formula through Quick Help by pressing the Normal button and close it by pushing again this button. The Quick Help functionality is the same for all distribution panels.

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LogNormal distribution

The density function of the LogNormal distribution has the following expression:

$$f(x) = \frac{1}{x \cdot \sigma \cdot \sqrt{2\pi}} \exp\left[\frac{-1}{2} \left[\frac{\ln(x) - \mu}{\sigma}\right]^2\right] \cdot \mathbf{1}_{(0,\infty)}(x)$$

for x in $(0, \infty)$.

Insert the information Name Normal Note Change the distribution and the parameters LogNormal Oe+000
Name Normale Note Change the distribution and the parameters LogNormal 0e+000 1e+000 0.658 0.658 0.658 0.658 0.658 0.001 - 0.999 LogNormal 0.564 0.376
Note Change the distribution and the parameters LogNormal 0e+000 1 0e+000 1 0e+000 1 0e+000 1 0.658 0.658 0.658 0.658 0.376
Change the distribution and the parameters LogNormal Image: Comparison of the parameters 0e+000 Image: Comparameters
LogNormal 0e+000 1e+000 0.658 0.658 0.658 0.658 0.658 0.658 0.001 - 0.999 LogNormal 0.658 0.376 0.376
0e+000 1e+000 0.658 0.658 0.658 0.658 0.658 0.001 - 0.999 LogNormal
1e+000 2 0.658 - LogNormal 0.564 - 0.470 - 0.376 - 0.376 - 0.470 - 0.470 -
0.658 0.564 0.470 0.376
0.658
0.564 - 0.470 - 0.376 -
0.376 - {
- (
0.282 - (
0.188
0.094
0.000 0.48 0.95 1.43 1.90 2.38 2.86 3.33 3.81
Apply Reset <u>O</u> K Cancel

Figure 90 Log-Normal distribution panel

Distribution parameters

 $\mathbf{1}$ μ parameter; the default value for μ is 0.

2 σ parameter; the default value for σ is 1.

3 Truncation value; the default value is in [0.001, 0.999].

Mean value: $\exp\left(\mu + \frac{1}{2}\sigma^2\right)$ Standard deviation: $\exp\left(2\mu + 2\sigma^2\right) - \exp\left(2\mu - \sigma^2\right)$

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Uniform distribution

The density function of the Uniform distribution has the following expression:

$$f(x) = \sum_{i=1}^{n} \frac{Weight_{i}}{RightVal_{i} - LeftVal_{i}}$$

with *n* number of intervals.

HI UniformDistribution	_	. 🗆 🗙
Insert the information		
Name Normale		
Noto		
Change the distributio	on and the parameters	
Uniform		
	Left Val Bight Val Weight	
2 SAVE)
	·	
1.000		
0.957	<u>. Un</u>	rorm
0.714 -		
0.571 —		
0.429 —		
0.286 —		
0.143 —		
0.000		
0.00 0.13	0.25 0.38 0.50 0.63 0.75 0.88 1.00	
<u>A</u> pply I	Reset <u>Q</u> K Cancel	

Figure 91 Uniform distribution panel

Buttons description 1 LOAD button. The user can select this button to load a set of intervals for the current uniform distribution. This list of intervals will overwrite any previous list of intervals present in the matrix.



3 ADD button. This button is used to insert a new interval for the current uniform distribution. For each interval, the user has to insert the left bound, the right bound and the relative weight of the interval. The intervals can't overlap and the sum of the weights must be equal to 1.

DEL button. With this button the user may delete any interval present in the matrix. The user must select one interval before pressing the DEL button. After deleting an interval, the weight of the remaining elements must be corrected.

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APPENDIX A

ParametersThis area contains the parameters that characterise the uniform distribution:areaRightVal $_i$ and LeftVal $_i$ are the extreme values of i-th subinterval so that

(RightVal_{*i*} - LeftVal_{*i*}) > 0 for each *i*;

Weight i is the weight of the i-th subinterval, the sum of all the weights must be equal to 1.

The user can modify each value double clicking the matrix item.

Mean Value:
$$\sum_{i=1}^{n} \left(\frac{LeftVal_{i} + RightVal_{i}}{2} \right) * w_{i}$$

Standard deviation:
$$\sqrt{\sum_{i=1}^{n} \left(\frac{(LeftVal_{i}^{3} - RightVal_{i}^{3})}{LeftVal_{i} - RightVal_{i}} * \frac{1}{3} * w_{i} \right)}$$

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LogUniform distribution

The density function of the LogUniform distribution has the following expression:

$$f(x) = \sum_{i=1}^{n} \frac{Weight_{i}}{x \cdot (\ln(RightVal_{i}) - \ln(LeftVal_{i}))}$$

with *n* number of intervals.

R LogUniformDistribution	_ 🗆 ×
Insert the information	
Name Normale	
Note	
Change the distribution and the parameters	
Left Val Right Val Weight	
LOAD 1.000000 2.718282 1.000000 A DEL	
1.000 0.857 0.714 0.571 0.429 0.286 0.143 0.000 1.00 1.21 1.43 1.64 1.86 2.07 2.29 2.50 2.72	LogUniform
Apply Reset <u>D</u> K	Cancel

Figure 92 LogUniform distribution panel

Mean Value (
$$\mu$$
): $\sum_{i=1}^{n} \frac{RightVal_{i} - LeftVal_{i}}{\log(RightVal_{i}) - \log(LeftVal_{i})}$

Standard deviation:

$$\sqrt{\sum_{i=1}^{n} \left(\frac{RightVal_{i}^{2} - LeftVal_{i}^{2}}{2 \cdot \left(\log(RightVal_{i}) - \log(LeftVal_{i})\right)}\right)} + \mu^{2} - 2\mu \cdot \frac{RightVal_{i} - LeftVal_{i}}{\log(RightVal_{i}) - \log(LeftVal_{i})}$$

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Distribution

parameters

Weibull distribution

The density function of the Weibull distribution has the following expression:

$$f(x) = \frac{\beta}{n} * \left[\frac{x-b}{n}\right]^{\beta-1} \cdot \exp\left[-\left(\frac{x-\beta}{n}\right)^{\beta}\right]$$



Figure 93 Weibull distribution panel

- **1** β value with $\beta > 0$; the default value for β is 1.
- **2** n value with n > 0; the default value for n is 1.
- **3** b value with $b \ge 0$; the default value for b is 0.
- Right truncation value; the default value is 0.999

Mean value:
$$n \cdot \Gamma\left(1 + \frac{1}{\beta}\right) + b$$

Standard deviation: $\sqrt{n^2 \cdot \left[\Gamma\left(1 + \frac{2}{\beta}\right) - \Gamma^2\left(1 + \frac{1}{\beta}\right)\right]}$

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Constant factor

The user may insert constant factors using this panel. Constant factors are excluded by the sample generation process.

88 Constant		_ 🗆 ×
Insert the information		
Name nonameConst		
Note		
Change the distribution and the parameters		
Constant		
Te+000 Value		
Reset	ОК	Cancel

Figure 94 Constant distribution panel

• This field specifies the value of the constant factor; the default value for a constant is 1.

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Exponential distribution

The density function of the Exponential distribution has the following expression:

```
f(x) = \lambda \cdot \exp\left[-\lambda \cdot (x-b)\right]
```

Exponential Distribution
Insert the information
Name Normale
Note
Change the distribution and the parameters
Exponential
1e+000 λ Right Truncation: 0.999
2 0е+000 ь
1.000 <u>Exponential</u> 0.857 <u>0</u> .714 <u>0</u> .571 <u>0</u> .429 <u>0</u> .286 <u>0</u> .143 <u>0</u> 0
0.000
Apply Reset <u>OK</u> Cancel

Figure 95 Exponential distribution panel

Distribution parameters

λ value with λ > 0; the default value for λ is 1.
b value with b > 0 and x ≥ b; the default value for b is 0.
Right truncation value; the default value is 0.999.

Mean value:
$$\frac{1}{\lambda} - b$$

Standard deviation: $\frac{1}{\lambda^2}$

Distribution parameters

Gamma distribution

The density function of the Gamma distribution has the following expression:

$$f(x) = \frac{\lambda^{\mathrm{r}}}{\Gamma(\mathrm{r})} * (x - \mathrm{b})^{\mathrm{r}-1} * \exp(-\lambda * (x - \mathrm{b}))$$

🗱 Gamma Distribution	
Insert the information	
Name Normale	
Note	
Change the distribution and the parameters	
Gamma	
1e+	Right Truncation 0.999
le+ λ	-
0e+000 b	
1.000 0.857 0.714 0.571 0.429 0.286 0.143 0.000 0.000 0.000 0.63 1.25 1.88 2.50 3.13 Аррly Reset	<u>G</u> amma 3.75 4.38 5.00 <u>OK</u> Cancel

Figure 96 Gamma distribution panel

- **1** r value with r > 0; the default value for r is 1.
- **2** λ value with $\lambda > 0$; the default value for λ is 1.
- **3** b value with $b \ge 0 \& x \ge b$; the default value for b is 0.
- **4** Right truncation value; the default value is 0.999.

Mean value: $\frac{r}{\lambda} + b$

Standard deviation: $\sqrt{\frac{r}{\lambda^2}}$

Beta distribution

The density function of the Beta distribution density function has the following expression:

$$f(x) = \frac{1}{B(\alpha, \beta)} * \frac{1}{b-a} * \left[\frac{x-a}{b-a}\right]^{\alpha-1} * \left[\frac{b-x}{b-a}\right]^{\beta-1}$$

🕷 BetaDistribution 📃 🗖 🗙
Insert the information
Name Normale
Note
Change the distribution and the parameters
Beta 💌
Ο 2e+000 α Β 0e+000 a
2e+000 β
1 500
1071 -
0.857 -
0.643 —
0.429 -
0.214 -
0.00 0.13 0.25 0.38 0.50 0.63 0.75 0.88 1.00
Apply Reset <u>D</u> K Cancel

Figure 97 Beta distribution panel

Distribution parameters

α value with α > 0; the default value for α is 2.
 β value with β > 0; the default value for β is 2.
 a value with a < b; the default value for a is 0.
 b value; the default value for b is 1.

Mean value:
$$\frac{\alpha}{\alpha + \beta} * (b - a)$$

Standard deviation: $\sqrt{\frac{\alpha * \beta}{(\alpha + \beta + 1) * (\alpha + \beta)^2} * (b - a)^2}$

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Triangular distribution

The density function of the Triangular distribution has the following expression:

$$f(x) = \begin{cases} \frac{2*(x-\alpha)}{(\beta-\alpha)*(\gamma-\alpha)} & \alpha \le x \le \beta \\ \frac{2*(\gamma-x)}{(\gamma-\beta)*(\gamma-\alpha)} & \beta \le x \le \gamma \end{cases}$$

🗱 Triangular Distribution	_ 🗆 ×
Insert the information	
Name Normale	
Note	
Change the distribution and the parameters	
Triangular	
1e+000	
2e+000	
1.000	<u>T</u> riangular
0.897	
0.571 -	
0.429 -	
0.286 -	
0.143	
0.000	1
0.00 0.25 0.50 0.75 1.00 1.25 1.50 1.75 2.	00
Apply Reset <u>Q</u> K	Cancel

Figure 98 Triangular distribution panel

Distribution parameters

 $\mathbf{0}$ α value; the default value for α is 0.

2 β value; the default value for β is 1.

3 γ value with $\alpha \le \gamma < \beta$ or $\alpha < \gamma$. $\le \beta$; the default value for γ is 0.5.

Height of β point (h): $\frac{2}{(\gamma - \alpha)}$

Mean

$$\frac{h}{3(\beta-\alpha)} \cdot \left[\beta^{3} - \alpha^{3}\right] - \frac{\alpha \cdot h}{2(\beta-\alpha)} \left[\beta^{2} - \alpha^{2}\right] + \frac{-h}{3(\gamma-\beta)} \left[\gamma^{3} - \beta^{3}\right] + \frac{1}{2} \left(\frac{\beta \cdot h}{(\gamma-\beta)} + h\right) \cdot \left[\gamma^{2} - \beta^{2}\right]$$

Standard deviation:

$$\left(\frac{h}{4(\beta-\alpha)}\left[\beta^{4}-\alpha^{4}\right]-\frac{\alpha\cdot h}{3(\beta-\alpha)}\left[\beta^{3}-\alpha^{3}\right]+\right.\\\left.+\frac{-h}{4(\gamma-\beta)}\left[\gamma^{4}-\beta^{4}\right]+\frac{1}{3}\left(\frac{\beta\cdot h}{\gamma-\beta}+h\right)\cdot\left[\gamma^{3}-\beta^{3}\right]-\mu^{2}\right)^{\frac{1}{2}}$$

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Relation

This panel represents a special case among the input factors selection panels; the user can create a relation between inputs factors using the expression editor.

Panel	8 Relation	
description	Insert the information	
L	Name Factor3	
	Note	
	Change the distribution and the pa	arameters
	Relation	
	Factors' list	Available operations
	Factor1 Factor2	acos() 7 8 9 / Pow () 4 5 6 * 1 2 3 - 0 . +
	Factor1*1.5	
	Apply Reset	OK Cancel

Figure 99 Relation panel

Factors list. This field shows the available inputs factors; by double clicking an input factor, it is possible to insert that factor in the expression visualized in 3.

Available operations. In this section of the panel the user can select some functions and basic operations to apply to the inputs factors. This section has the same functionality of a calculator with field 3 as display.

Expression field. This field displays the current expression; it is possible to insert the expression through "Available operations" or directly through the keyboard.

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Discrete distribution

The density function of the discrete distribution has the following expression:

$$f(x) = Weight_i I_{(x_1..x_n)}$$

where $I_{(x_1,x_2)}$ is 1 in the x's points 0 otherwise.

Discrete Distribution				
Insert the information				
Name noname1				
Note				
Change the distribution	on and the para	meters		
Discrete	-			
	-		т	
•	Val	Weight]	ß
LOAD	0.000000	0.260000	▲ <u>A</u>	
SAVE	0.500000	0.300000		9
	1 000000	0.240000	-	
0.360 —				Discrete
0.309 —				
0.257 —				
0.206 —		•		
0.154 —				
0.103 —				
0.051 —				
0.000				1
-0.10 0.05	0.20 0.35 0.	50 0.66 0.8	1 0.96 1.	11
<u>Apply</u> F	Reset			Cancel

Buttons description

Figure 100 Uniform distribution panel

ULOAD button. The user can select this button to load a set of points for the current discrete distribution. This list of points will overwrite any previous list of points present in the matrix.

2 SAVE button. This button allows the user to save in a file the current points for the discrete distribution.

3 ADD button. This button is used to insert a new point for the current discrete distribution. For each interval, the user has to insert the value of the point and the relative weight of the point. Points can't overlap and the sum of the weights must be equal to 1.

4 DEL button. With this button the user may delete any point present in the matrix. The user must select one interval before pressing the DEL button. After deleting an interval, the weight of the remaining elements must be corrected.

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ParametersThis area contains the parameters that characterise the discrete distribution.areaWeight $_i$ is the weight of point i the sum of weights must be equal to 1.

By double clicking an item in the 'Parameters area' the user can modify its value .

Mean Value: $\sum_{i=1}^{n} w_i * x_i$ for each x in which the distribution is defined

Standard deviation: $\sqrt{\sum_{i} (x_i - \mu_x)^2 * w_i}$

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APPENDIX B: DEFINITIONS OF INTERACTION MEASURES IN EE METHOD AND NOTES

INTERACTION EFFECTS IN MORRIS GRAPHS



OUR PROPOSAL (Muñoz-Carpena, 2007; Chu-Agor et al., 2011) (for μ*)



OTHER NOTES - Number of model runs (from Saltelli et al., 2004)

N= number of samples; k = number of factors; M is the sample size in the MonteCarlo simulation, N \approx 500/1000; r is no. Morris trajectories, generally sufficient at r=10 (Campolongo et al., 1997)

Sobol: Original (Simlab v2.2) N= (2k + 2)M; Mod. Sobol (R pkg, Saltelli, 2002) N=(K+2)M FAST: N \approx kM Morris: N=r(k + 1)

Example: k = 20 --> N_{Sobol1} = 21000 -42000; N_{Sobol2} = 11000 -22000 ; N_{FAST} = 10000-20000 ; N_{Morris} = 210

APPENDIX C: INPUT FACTORS FILE FORMAT (.FAC) © SIMLAB V2.2.1, EU JCR ISPRA

APPENDIX C

This section describes the file formats that are created during the SimLab working sessions.

INPUT FACTORS FILE FORMAT (.FAC)

Input factors are generated in the first step of the Monte Carlo analysis. For each factor the user selects a range and a distribution type with distribution specific parameters; these information are saved in a file having *fac* extension.

The *fac* file contains the following information:

default truncations values that the user can change using the default truncations window;

total number of inputs factors;

then, for each input factor, the file contains:

factor type; factor name; factor notes;

factor specific parameters (dependent on the factor type).

Again, for each factor, is listed the relative dependence tree correlation information:

Dependence tree correlation value for the factor;

Dependence tree parent of the factor in the correlation tree (-1 for item without parents);

number of children in the dependence correlation tree;

for each child: his **position** in the list of factors;

all the values in the Iman Conover correlation matrix.

Stein correlatin information

The correlation method selected by the user: 0 dependence tree, 1 Iman Conover, 2 stein correlation 3 no correlation

The following is an example of a file *.fac*:

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Figure 110 fac file example

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