

Design of Experiments and Sensitivity analysis

Course and practical application

eX Modelo Summer School

OpenMOLE

August 31st, 2020

- ▶ Interactive model exploration by hand and the need for preliminary experiments
- ▶ The Design of Experiments (DOE) as the definition of computational experiments to extract information from the simulation model
- ▶ Example: NetLogo behavior space: basic grid DOE
- ▶ Sensitivity analysis as an advanced DOE

Remark 1: *terminology strongly depends on disciplines and practices*

Remark 2: *most are generally **preliminary experiments** to prepare more elaborated, question-related, experiments*

- 1 Basic experiments
- 2 High-dimensional samplings
- 3 Sensitivity analysis

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*Provide explicitly sampling points on which the model (or its replication task) will be run: notion of **direct sampling** in OpenMOLE (corresponds to DOE in the literature)*

- ▶ full samplings
- ▶ elaborated sampling for high dimensions given a low computational budget (**the curse of dimensionality**)

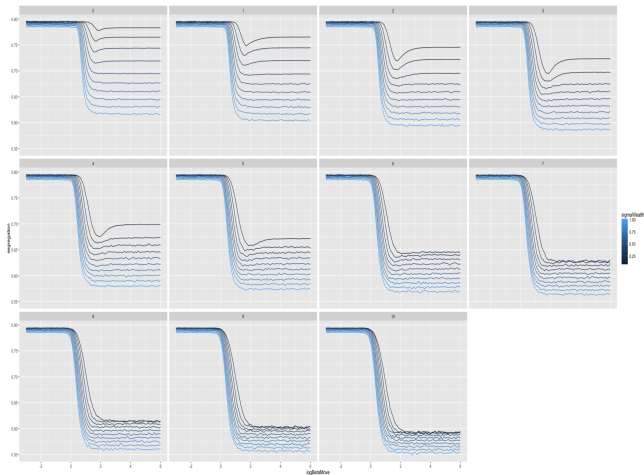
Syntax of the direct sampling method in OpenMOLE:

```
val explo = DirectSampling(  
  evaluation = (model hook reshock on env by 500),  
  sampling =  
    (humanFollowProbability in (0.0 to 1.0 by 0.1))  
    x (humanInformedRatio in (0.0 to 1.0 by 0.1))  
    x (humanInformProbability in (0.0 to 1.0 by 0.1))  
    x (replication in UniformDistribution[Long](100000) take 100)  
)
```

Cheapest and intuitive DOE: *all factors have nominal values and a discrete variation set, in which each is varied while others remaining fixed*

- ▶ when model is slow - or computational budget highly limited
- ▶ does not capture interaction between parameters, and highly dependent on nominal values
- ▶ seen as a bad practice **BUT** useful for models taking significant time, and prone to thematic interpretation

Example where One-At-a-Time fails



Indicator variations in a 3D parameter space: some nominal values make non-monotonous effects disappear

Brute force DOE: *ensemble product of discrete variation ranges for factors (usually a regular grid but not necessarily)*

- ▶ quickly limited by the curse of dimensionality - in practice still powerful with a quick model and a low number of parameters
- ▶ naive approach, but remains only DOE for many "simulation-newcomers" disciplines

One-factor sampling:

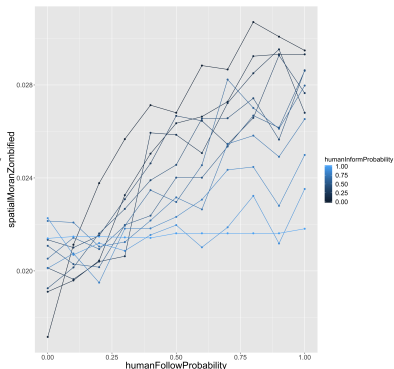
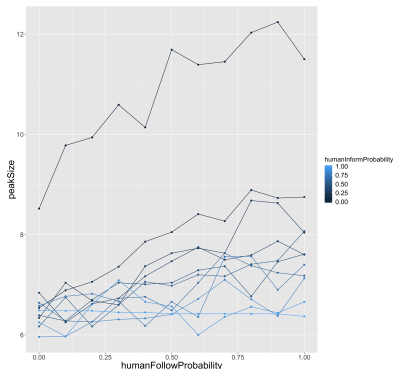
```
sampling = OneFactorSampling(  
    (x1 in (0.0 to 1.0 by 0.2)) nominal 0.5,  
    (x2 in (0.0 to 1.0 by 0.2)) nominal 0.5  
)
```

Grid sampling:

```
sampling =  
    (x1 in (0.0 to 1.0 by 0.5)) x  
    (x2 in (0.0 to 1.0 by 0.5))
```

- ▶ Given the described zombie model, what first experiment beyond stochasticity would be relevant ?
- ▶ Explore and test the `directsampling.oms` script available in the downloaded archive (see chat for link)

Regular grid sampling for the three parameters of the basic ZOMBIE model, with 100 replications



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Computational limitations \implies need specific methods to efficiently sample the parameter space

Different methods for improving sampling in numerical experiments given limited computational resources have been proposed, as for example:

- ▶ Sobol sequences (quicker convergence of for Monte Carlo estimation of integrals)
- ▶ Latin Hypercube Sampling
- ▶ Orthogonal sampling

Minimizing discrepancy for a point cloud: intuitively being spread evenly across the definition space

L2-discrepancy given for normalized data points $\mathbf{X} = (x_{ij}) \in [0, 1]^d$ by

$$\left\| \mathbf{t} = (t_j) \in [0, 1]^d \mapsto \frac{1}{n} \sum_i \mathbb{1}_{\prod_j x_{ij} < t_j} - \prod_j t_j \right\|_2$$

Explanation: $\prod_j t_j$ is the volume of the hypercube between \mathbf{t} and the origin; the sum of indicator functions counts the points within that hypercube; the difference between expected volume and point number is integrated over the whole hypercube.

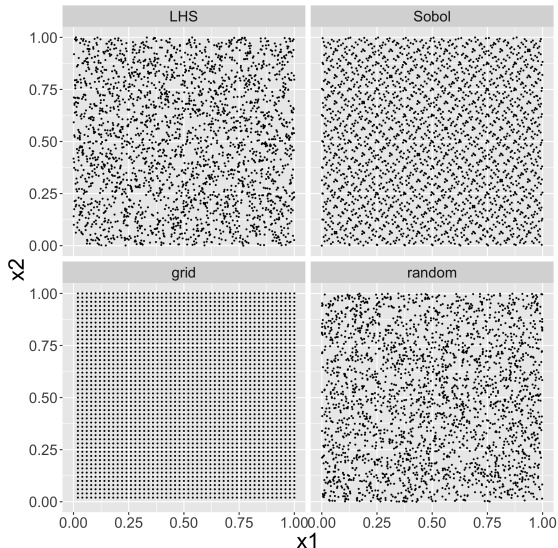
x				
	x			
				x
			x	
		x		

Latin cube: one point in each row and column; hypercube generalization in any dimension

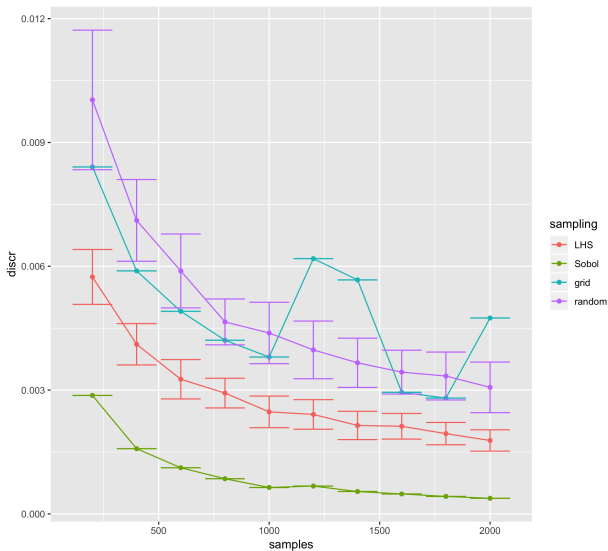
Sobol sequences are a case of quasi-random sequences with low discrepancy (also Halton sequences e.g.)

- ▶ Estimate integrals in $1/N$ instead of $1/\sqrt{N}$ with random sampling
- ▶ Constructed recursively (using bit representations)

For $N = 2500$ samples in 2 dimensions



Estimated discrepancies for repetitions of samplings as a function of sample size



LHS Sampling

```
sampling = LHS(  
    100,  
    x1 in (0.0,1.0),  
    x2 in (0.0,1.0)  
)
```

Sobol sampling

```
sampling = SobolSampling(  
    100,  
    x1 in (0.0,1.0),  
    x2 in (0.0,1.0)  
)
```

→ **Practice:** test these samplings in `directsampling.oms`

Summary of samplings characteristics

	Coverage	Interpretability	Budget
One factor at a time	✗	✓	✓
Complete plan	✓	✓	✗
LHS/Sobol	✓	✗	✓

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Aim of sensitivity analysis methods *How to summarize model sensitivity and isolate principal factors ?*

- ▶ Most methods are *global*, i.e. provide an aggregate of factor effect on the full parameter space
- ▶ Advanced methods, still useful for preliminary experiments e.g. to discard factors from further experiments
- ▶ Examples: Morris and Saltelli methods

Idea: *Sample trajectories in the parameter space in a One-At-a-Time manner. Screening method isolating **elementary effects***

- ▶ isolate local effects of factors
- ▶ more efficient than point sampling to get individual effects
- ▶ useful as a first experiment to understand the relative influence of factors

Introduced by [Morris, 1991], improved by [Saltelli et al., 2004], [Campolongo et al., 2011] propose to extend the method with Sobol sequences

Let δ be step for parameter variation (all assumed normalized in $[0; 1]$), the *elementary effect* for parameter i on output Y at point \vec{x} is given by

$$\varepsilon_i(\vec{x}) = \frac{Y(\vec{x} + \delta \cdot \vec{e}_i) - Y(\vec{x})}{\delta}$$

With N parameter trajectories randomly sampled (each trajectory varying all parameters), the sensitivity index is given by

$$\mu_i = \frac{\sum_{k=1}^N \varepsilon_i(\vec{x}_k)}{N}$$

and complementary indices by

$$\sigma_i = \frac{\sum_{k=1}^N (\varepsilon_i(\vec{x}_k) - \mu_i)^2}{N}$$

$$\mu_i^* = \frac{\sum_{k=1}^N |\varepsilon_i(\vec{x}_k)|}{N}$$

In OpenMOLE, Morris is a method in itself (and not a sampling)

```
SensitivityMorris(  
  evaluation = (model on env by 5000),  
  inputs = List(  
    humanFollowProbability in (0.0,1.0),  
    humanInformedRatio in (0.0,1.0),  
    humanInformProbability in (0.0,1.0)  
  ),  
  outputs = List(totalZombified,halfZombified),  
  repetitions = 1000,  
  levels = 20  
) hook CSVHook(workDirectory / "morris_result.csv")
```

→ **Practice:** explore the script `morris.oms`, comment the results obtained with a large-scale experiment `morrisresults`

Method based on the estimation of conditional relative variances
[Saltelli et al., 2010]

First order index

$$S_i = \frac{\text{Var}[E_{\mathbf{X}_{\sim i}}(Y|X_i)]}{\text{Var}(Y)}$$

is the expected relative variance reduction if X_i would be fixed

Total effect index

$$ST_i = \frac{E_{\mathbf{X}_{\sim i}}[\text{Var}(Y|\mathbf{X}_{\sim i})]}{\text{Var}(Y)}$$

is the expected relative variance if all factors but X_i are fixed
(includes interaction effects)

In OpenMOLE, Saltelli is also a method

```
val sen = SensitivitySaltelli(  
  evaluation = (model on env by 1000),  
  samples = 100000,  
  inputs = List(  
    humanFollowProbability in (0.0,1.0),  
    humanInformedRatio in (0.0,1.0),  
    humanInformProbability in (0.0,1.0)  
  ),  
  outputs = List(totalZombified,halfZombified)  
)  
  
sen hook SaltelliHook(sen,workDirectory)
```

Summary of sensitivity methods

	Coverage	Interpretability	Budget
Morris	✗	✓	✓
Saltelli	✓	✓	✗

Take-home messages:

- ▶ Direct sampling can be useful as preliminary experiments, but also experiments in themselves
- ▶ Sensitivity analysis methods are useful for a global knowledge on influence of factors
- ▶ Find a good balance interpretability/computational budget/information extracted
- ▶ The experiments you choose depend on your questions but also on your discipline



Campolongo, F., Saltelli, A., and Cariboni, J. (2011).
From screening to quantitative sensitivity analysis. a unified
approach.
Computer Physics Communications, 182(4):978–988.



Morris, M. D. (1991).
Factorial sampling plans for preliminary computational
experiments.
Technometrics, 33(2):161–174.



Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M.,
and Tarantola, S. (2010).
Variance based sensitivity analysis of model output. design and
estimator for the total sensitivity index.
Computer Physics Communications, 181(2):259–270.



Saltelli, A., Tarantola, S., Campolongo, F., and Ratto, M. (2004).

Sensitivity analysis in practice: a guide to assessing scientific models.

Chichester, England.