Design of Experiments and Sensitivity analysis

Course and practical application

eX Modelo Summer School

OpenMOLE

June 31st 2021

- 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*

Outline

Basic experiments

*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:

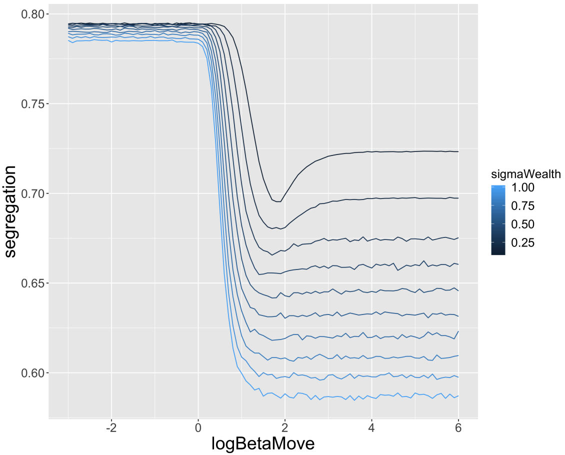
```
DirectSampling(
  evaluation = model,
  sampling =
      (humanFollowProbability in (0.0 to 1.0 by 0.5))
    x (humanInformedRatio in (0.0 to 1.0 by 0.5))
    x (humanInformProbability in (0.0 to 1.0 by 0.5))
    x (seed in UniformDistribution[Long](100000) take 100)
)
```

One factor at a time

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

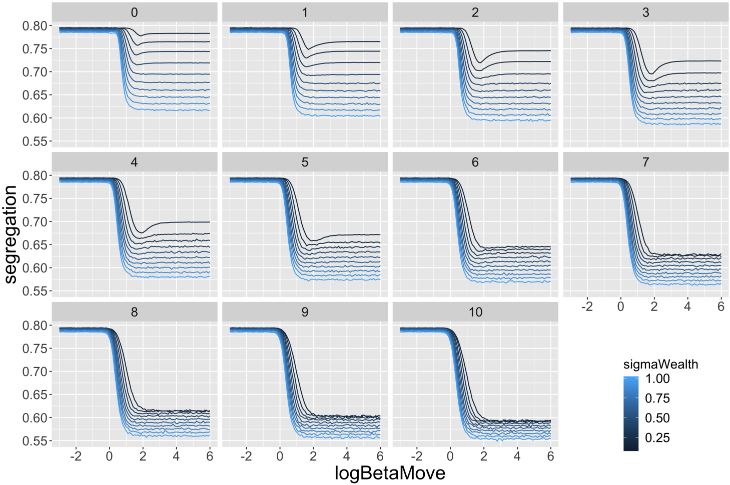
Example where One-At-a-Time fails



Indicator variations in a 2D parameter space: some nominal values for the colour parameter make non-monotonous effects with the first parameter disappear

Example where One-At-a-Time fails

OpenMOLE



Adding a dimension makes the effect even more difficult to get

Grid sampling

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:

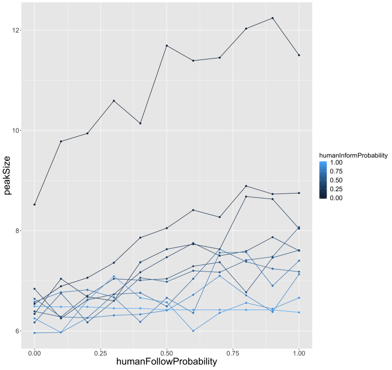
```
sampling =
     (x1 in (0.0 to 1.0 by 0.5)) x
     (x2 in (0.0 to 1.0 by 0.5))
```

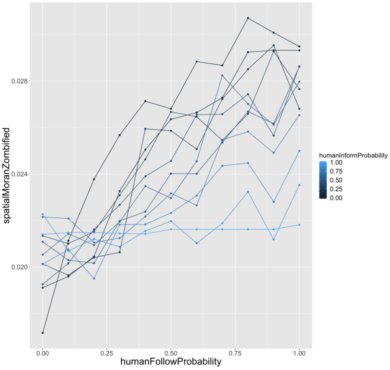
Practical application

OpenMOLE

- Given the described zombie model, what first experiment beyond stochasticity would be relevant?
- Explore and test the `1_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





High-dimensional samplings

Computational limitations $\Longrightarrow$ *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

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

L2-discrepancy given for normalised 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.*

Latin Hypercube Sampling

X				
	X			
				X
			X	
		X		

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

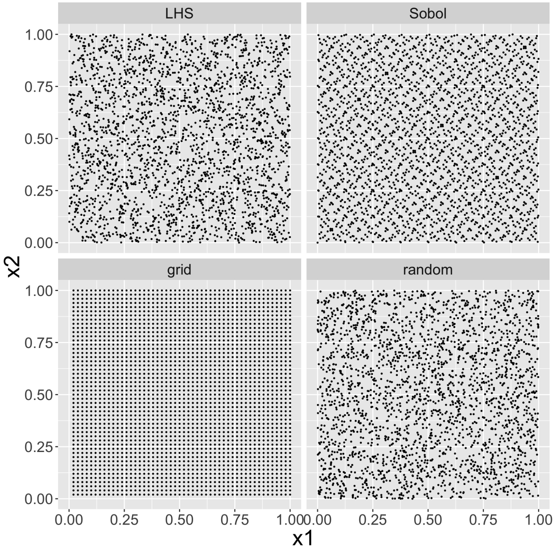
Sobol sequence

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)

Comparison of samplings

For $N = 2500$ samples in 2 dimensions



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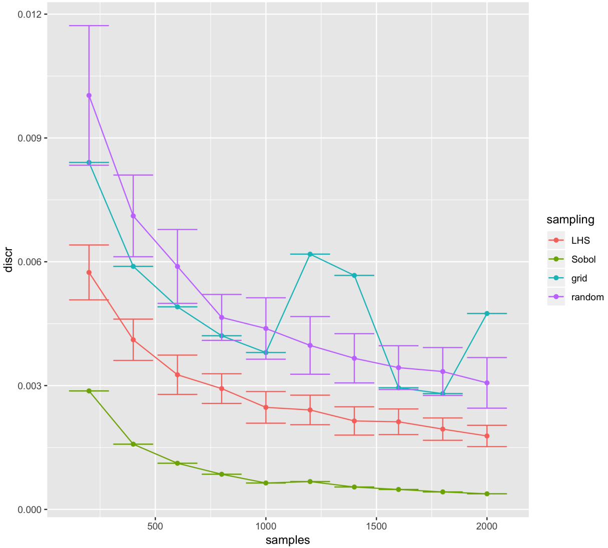
Estimated discrepancies for repetitions of samplings as a function of sample size



Syntax of high-dimensional samplings

LHS Sampling

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

Sobol sampling

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

→ **Practice:** test these samplings in `1_directsampling.oms`

Summary of samplings characteristics

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

Aim of sensitivity analysis methods *How to summarise 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

Morris method

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,
  inputs = Seq(
    humanFollowProbability in (0.0, 1.0),
    humanInformedRatio in (0.0, 1.0),
    humanInformProbability in (0.0, 1.0)
  ),
  outputs = Seq(totalRescued, totalZombified, peakTime, peakSize),
  sample = 1000,
  level = 20
) hook (workDirectory / "morris_result")
```

→ **Practice:** explore and run the script `2_morris.oms`

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

First order index

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

is the expected relative variance reduction if X_i would be fixed

Total effect index

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

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

In OpenMOLE, Saltelli is also a method

```
SensitivitySaltelli(
  evaluation = model,
  inputs = Seq(
    humanFollowProbability in (0.0, 1.0),
    humanInformedRatio in (0.0, 1.0),
    humanInformProbability in (0.0, 1.0)
  ),
  outputs = Seq(totalRescued, totalZombified, peakTime, peakSize),
  sample = 10,
) hook (workDirectory / "saltelli_result")
```

OpenMOLE

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

References I

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.