Sensitivity Analysis

How to perform comprehensive, efficient, and robust Sensitivity Analysis?

Dr. Debraj Roy

Computational Science Lab, University of Amsterdam

Table of contents

Introduction

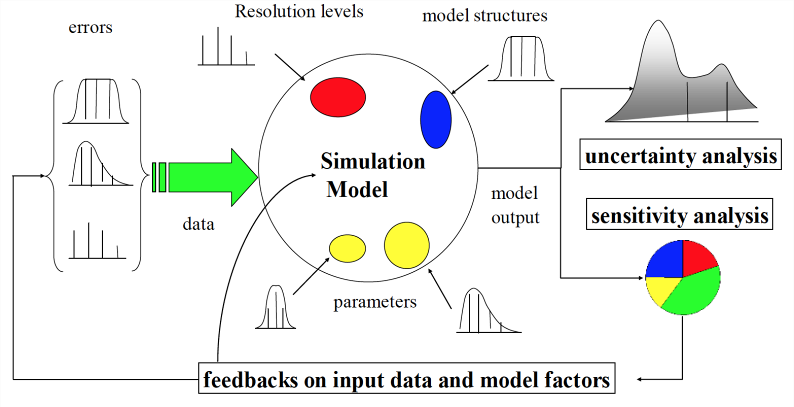
Modelling & Simulation

"Essentially, all models are wrong, but some are useful."

— Box, George E. P.; Norman R. Draper (1987). Empirical Model-Building and Response Surfaces, p. 424, Wiley. ISBN 0471810339.

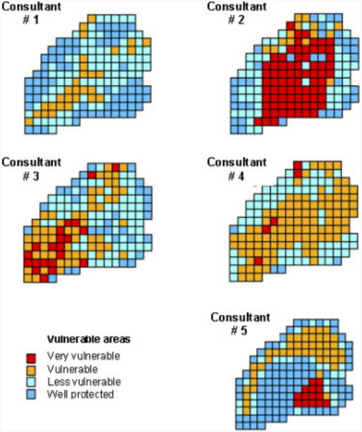
Uncertainty analysis: Focuses on just quantifying the uncertainty in model output.
Sensitivity analysis: The study of the relative importance of different input factors on the model output.

Modelling & Simulation



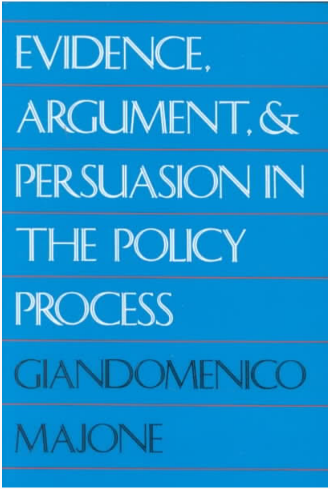
Modelling & Simulation

key question: which parts of this particular area are most vulnerable to pollution and need to be protected?



Refsgaard, Jens Christian, Jeroen P. Van der Sluijs, James Brown, and Peter Van der Keur. "A framework for dealing with uncertainty due to model structure error." Advances in Water Resources 29, no. 11 (2006): 1586-1597.

"Are the results from a particular model more sensitive to changes in the model and the methods used to estimate its parameters, or to changes in the data?"



What is the issue

- Models in ecology, social simulation, etc. contain parameters with uncertain estimates
- This, in turn, leads to uncertain model outcomes
- How the model outcomes respond to changes in input parameters is typically not known
- How to analyse model behaviour?

Sensitivity Analysis

[Global*] **sensitivity analysis**: "The study of how the uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input"

Saltelli A., 2002, Sensitivity Analysis for Importance Assessment, Risk Analysis, 22 (3), 1-12.

Aims of sensitivity analysis

- Assess uncertainty of model outcomes
- Identifying influential parameters
  - Establish research priorities
- Hypothesis testing
  - Do the model mechanisms present a good explanation for real-life observations?
- Testing robustness of model findings
- Gaining a better understanding of model behaviour

Applications of sensitivity analysis

Factor prioritization
which factors determine output the most

Factor fixing
which factors can be removed from the model

Variance cutting
which factors, made more certain, would make output more certain

Factor mapping
which factors are most important for causing good/bad outputs

Applications of sensitivity analysis

Impact assessment guidelines: what do they say about sensitivity auditing ?

Better Regulation "Toolbox"

This Toolbox complements the Better Regulation Guideline presented in in SWD(2015) 111

It is presented here in the form of a single document and structured around various chapters containing individual tools. It is also available and intended to be used as a series of web-tools which are downloadable from the Commission's Better Regulation web site. http://ec.europa.eu/smart-regulation/index_en.htm

The Toolbox presents a comprehensive array of additional guidance to assist practitioners in the application of Better Regulation. Users are not expected to read and apply each individual tool but to use the toolbox selectively and with common sense.

Questions about this toolbox can be sent to units C1, C2, C3 and C4 of Directorate responsible for Smart Regulation and the Work Programme in the Secretariat General.

Types of sensitivity analysis

- Sensitivity analysis (SA) : quantification of the effects of changes or uncertainties in a models input parameters on the model output
    - Local SA: Consider only the effect of changes in individual parameters
    - Global SA: Consider the effects of changes in multiple parameters simultaneously

Local Sensitivity analysis

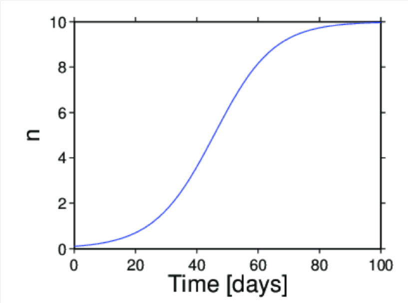
Which parameters when nudged will change the output most?

$$\left.\frac{\partial Y}{\partial X_i}\right|_{X^0}$$

Ricker model

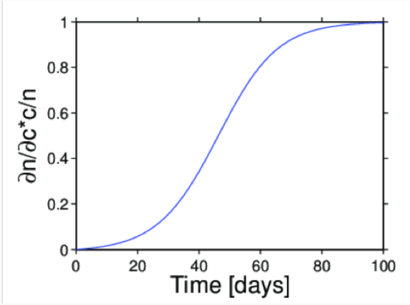
$$N_{t+1} = N_t e^{q(1-\frac{N_t}{c})}; N_0 = n_0$$

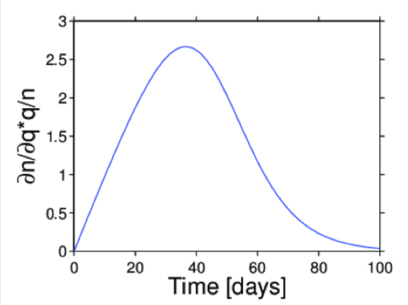
q : growth rate; c : carrying capacity



Ricker model

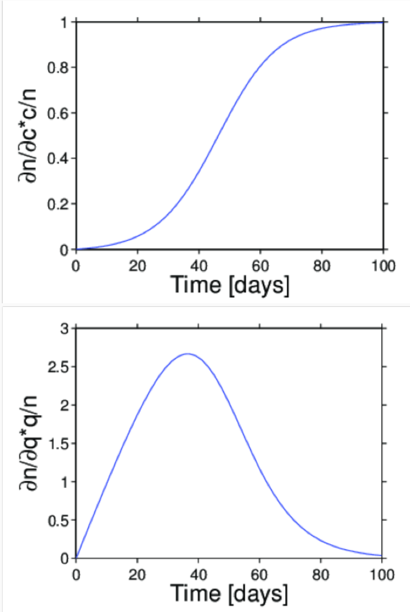
- Partial derivatives $\frac{\partial N}{\partial q}$, $\frac{\partial N}{\partial c}$ show how the output depends on parameters
- These were normalised for comparison





Ricker model

- Local sensitivity analysis shows which parameters are influential as function of time.
- Only holds for small parameter changes around default set.

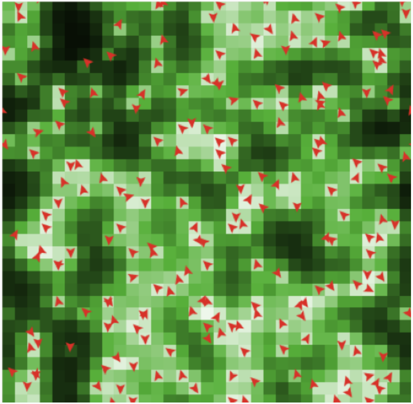


Local SA in Agent-based Model

- Several factors complicate analysis of ABMs
    - Nonlinear interactions and feedbacks
    - Different levels of input/output
    - Path-dependency
    - Stochasticity
    - Adaptivity
- We introduce a simple ABM to test this

Test Case Description

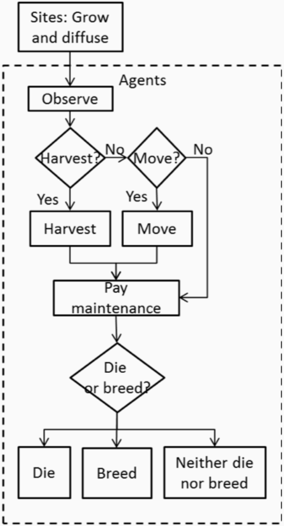
- Spatial consumer-resource system
- Square lattice, updated in discrete time-steps
- Resource :
  - Grows on sites
  - Diffuses between sites
- Agents (consumers) :
  - Need energy
  - Harvest resource for energy



Ten Broeke, G., Van Voorn, G., & Ligtenberg, A. (2016). Which sensitivity analysis method should I use for my agent-based model?. Journal of Artificial Societies and Social Simulation, 19(1), 5.

Test Case Description

- All decisions are stochastic
- Agents tend to harvest if :
  - internal energy is low
  - resource is abundant
  - other agents are close
- Agents move to sites with :
  - abundant resource
  - few agents



Flow chart for one time step

Input Parameters

- recommended to include all input parameters
- parameters may have different dimensions

Parameter	Description
c	Efficiency
D	Diffusion coefficient
E_b	Birth energy
E_h	Harvest cost
E_m	Cost of energy maintenance
E_{move}	Move cost
K	Carrying capacity
n_0	Initial number of agents
r	Growth rate
R_0	Initial resource
R_{max}	Maximum harvest
R_{unc}	Uncertainty of resource estimations
v_b	Birth coefficient
v_d	Mortality coefficient
z	Variation in offspring traits

Output Parameters

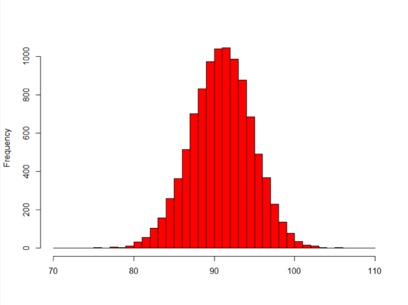
- As main output, we consider the number of agents n
- ABMs produce large amounts of outputs on different levels (e.g., system level, agent level)
- Multiple outputs may be considered separately during sensitivity analysis

Default parameter setting

- First step in most SA methods is to choose a default parameter setting
- This setting acts as a reference point to assess the effects of parameter changes
- First, we run the model a number of times in the default setting

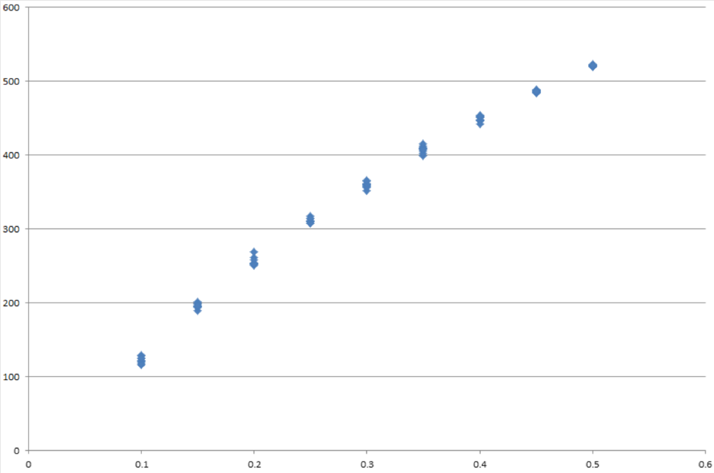
Histogram model runs

- The distribution resembles a normal distribution
- A large number of replicates is needed to estimate this distribution



One-factor-at-a-time (OFAT) SA

OAT results of r (resource growth rate)



OAT results of r (resource growth rate)

- The spread within replicates is small compared to the spread between replicates (i.e. stochasticity has little influence).
- The effect of the parameter on the output is approximately linear

One-at-a-time (OAT) designs

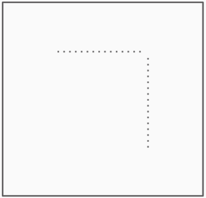
One parameter *changed* at a time

Pros:

In every pair, it's that parameter.

Easy.

Only 2 points per parameter (fixable - Elementary Effects method)



(hypercube in general)

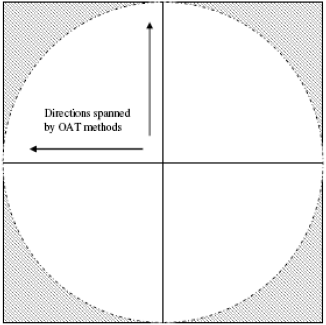
OAT is inefficient

Can we analyse influence of many parameters using few points?

3 points for each of 2 parameters. Parameter effects are mixed (but maybe we can un-mix them)

Homework: Analyse This?

OAT in 2 dimensions

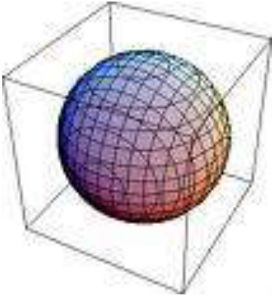


Area circle / area square =?

~ 3/4

Homework: Analyse This?

OAT in 3 dimensions



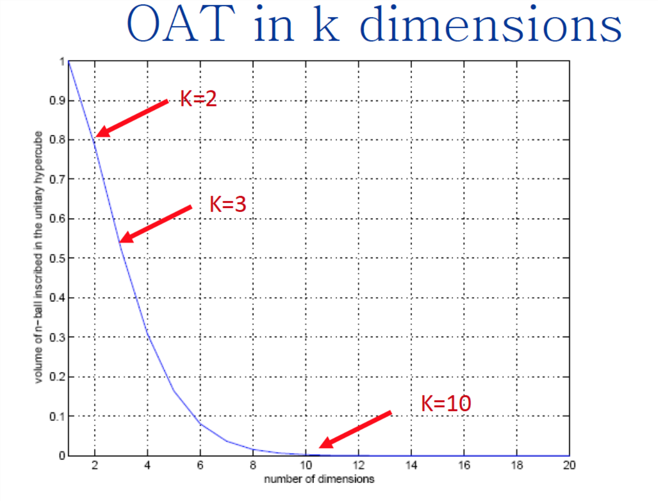
Volume sphere /
volume cube =?

~ 1/2

OAT in 10 dimensions

Volume hypersphere / volume ten dimensional hypercube =? ~ 0.0025

Homework: Analyse This?

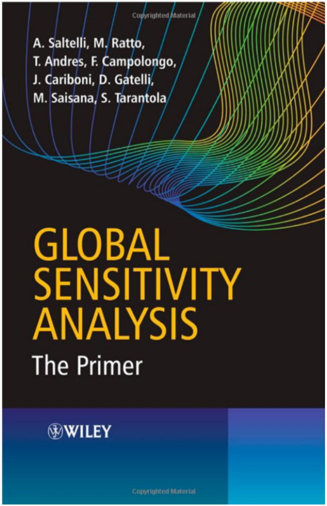


Conclusions on OFAT

- OFAT is a good method for analysing the qualitative behaviour of your ABM
- It can detect tipping points, and other non-linearities
- OFAT presents a good trade-off between costs (time) and gains (model insight) for ABM goals
    - Parameter effects are not readily comparable due to differences in dimensions and units
    - No interaction effects covered

Global Sensitivity analysis

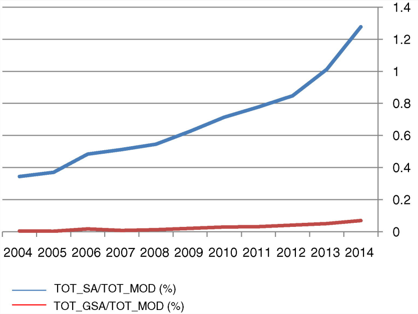
Global Sensitivity Analysis (GSA)

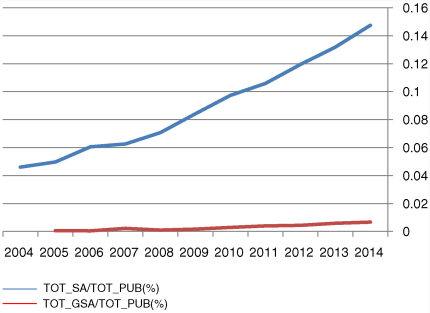


http://www.amazon.com/dp/0470059974/

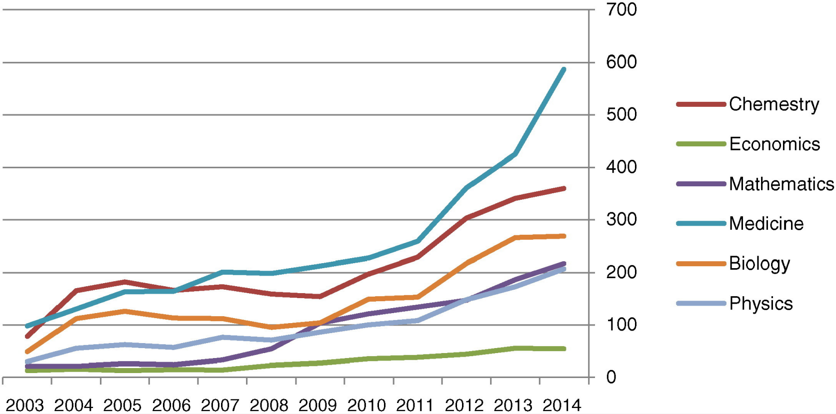
Which parameters are most significant over the entire input range?

Current state of art





Current state of art



Ferretti, F., Saltelli A., Tarantola, S., 2016, Trends in Sensitivity Analysis practice in the last decade, Science of the Total Environment, http://dx.doi.org/10.1016/j.scitotenv.2016.02.133

Decomposing models

$Y(X) = \sum_i f_i(X_i)$

Additive models easiest to analyse

Can we decompose the model itself into parts attributable to different parameters?

Decomposing models

$Y(X) = \prod_i f_i(X_i) \Leftrightarrow log\, Y(X) = \sum_i log\, f_i(X_i)$

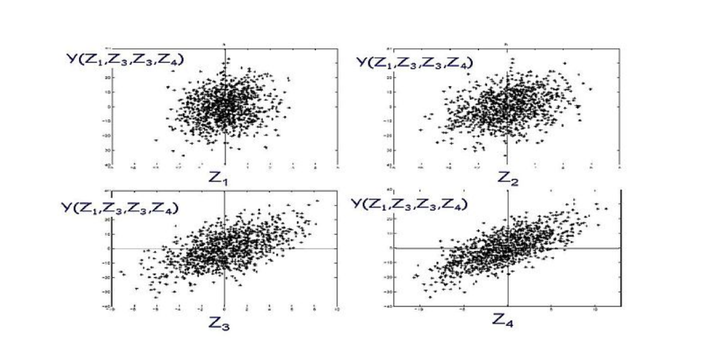
Not all models are additive. Some can be made additive.

Decomposing models

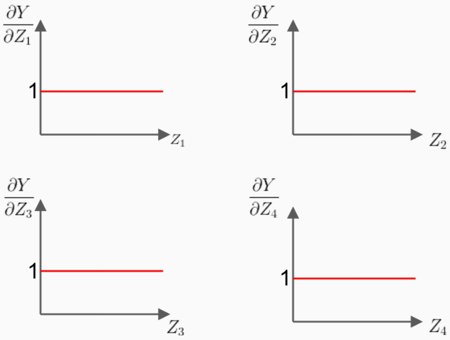
$Y = X_1^2 + X_2 X_3$

Ok, many models are actually more complex.

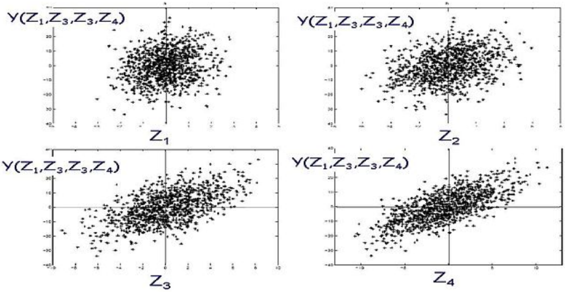
Can you guess the formula of Y?



Can you guess the formula of Y?



Can you guess the formula of Y?



Then why is Y more sensitive to Z3 and Z4?
Because they are more uncertain and contribute more to uncertainty of Y.
This emphasizes why variance is an important thing when analysing sensitivity, and why uncertainty of inputs matters just as much as the shape of the function.

Can you guess the formula of Y?

$\beta_i = \frac{\sigma_{X_i}}{\sigma_Y} \frac{\partial Y}{\partial X_i}$ larger input variance more sensitivity
$\sum_i \beta_i^2 = 1$ (looks like a decomposition of sensitivity)
That's why people measure sensitivity of linear functions not by dY/dX, but by scaling proportionally to standard deviation of input.
For a linear dependency, this will add up to 1 and give a decomposition of the strength of Y's dependency on each X.

Variance based methods

Attribute variance of output to different inputs and their interactions.

Fraction of variance explained

Before we describe the methods, let's talk more about what "fraction of explained variance" means.
$V(Y) = V^{explained\ by\ X_i} + V^{within\ X_i}$

Law of total variance

$V(Y) = E(V(Y \mid X)) + V(E(Y \mid X))$
$V(Y) = \sum_i V(E(Y|X_i))$ (for additive models)

Fun fact: for linear models, sensitivity computed this way is exactly the sigma-normalized derivative.
$S_i = \frac{V(E(Y|X_i))}{V(Y)}$

$\sum_i S_i = 1$

$S_i = \beta_i = \frac{\sigma_{X_i}}{\sigma_Y} \frac{\partial Y}{\partial X_i}$

$\sum_i S_i < 1$ (For non-additive models) $V(Y) = \sum_i V(E(Y|X_i)) +$???

Sobol decomposition aka HDMR

Remember this:

high-dimensional model representation

$Y = f_0 + \sum_i f_i(X_i) + \sum_{i,j} f_{ij}(X_i, X_j) + \dots$

Attributes parts of model to each combination of parameters.

Exists & unique if terms have zero mean

Sobol decomposition aka HDMR

$f_0 = E(Y)$

$f_i(x_i) = E(Y|X_i = x_i) - f_0$

$f_i(x_i, x_j) = E(Y|X_i = x_i, X_j = x_j) - f_i(x_i) - f_j(x_j) - f_0$
If parameters are independent, V distributes over this!

Variance decomposition

And now, the formula which makes everything work.
$V(Y) = \sum_i V(Y|X_i) + \sum_{i,j} V(Y|X_i, X_j) + \dots$

How is global sensitivity analysis done?

Setup for GSA

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & \dots & x_{1n} \\ x_{21} & x_{22} & x_{23} & \dots & x_{2n} \\ \multicolumn{5}{c}{\dotfill} \\ x_{d1} & x_{d2} & x_{d3} & \dots & x_{dn} \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{bmatrix}$$

Input matrix:

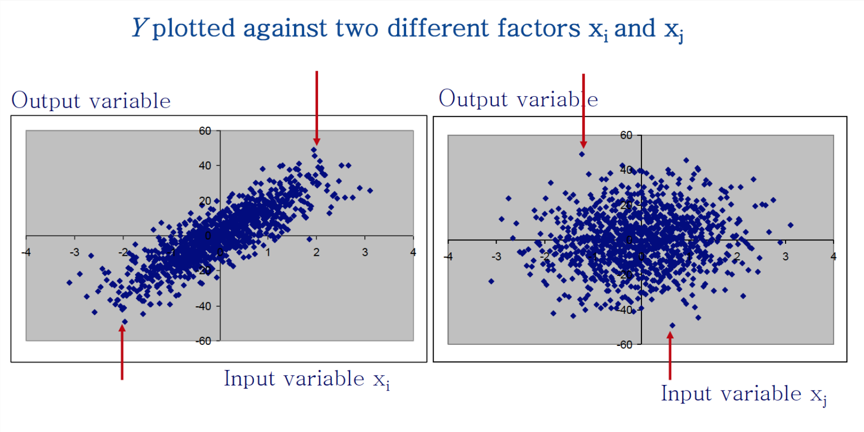
- Each column is a sample from the distribution of a factor.
- Each row is a sample trial to generate a value of y

Setup for GSA

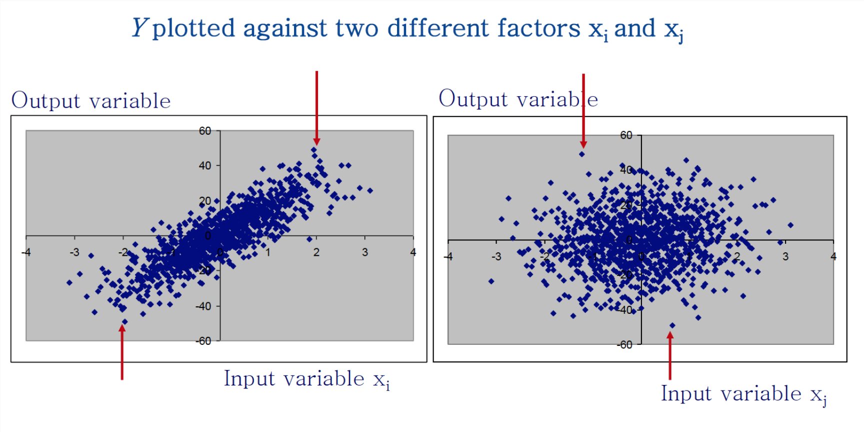
$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & \dots & x_{1n} \\ x_{21} & x_{22} & x_{23} & \dots & x_{2n} \\ \hdotsfor{5} \\ x_{d1} & x_{d2} & x_{d3} & \dots & x_{dn} \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_d \end{bmatrix}$$

Output vector:

- Just one output of interest; but y could also be a vector (function of time) or a map, etc. Each column is a sample from the distribution of a factor.
- y can be plotted against any of the x_i

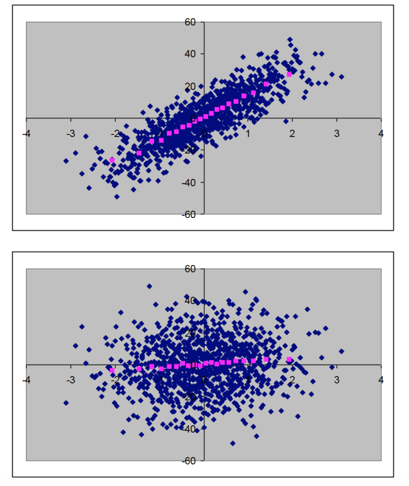


Can I do a sensitivity analysis just looking at the plots?



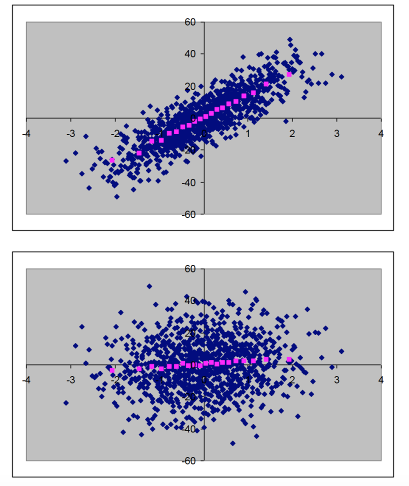
Which factor is more important? Why?

- 1,000 blue points
- Divide them in 20 bins of 50 points
- Compute the bins average (pink dots)



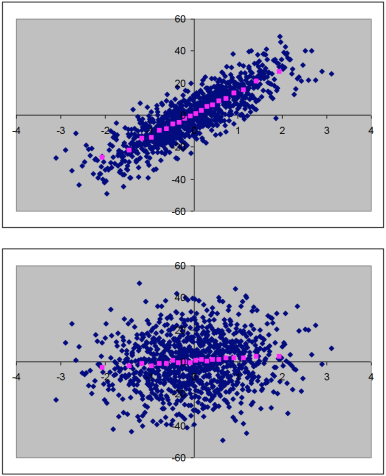
Each pink point is $E_{X_{\sim i}}(Y|X_i)$

- 1,000 blue points
- Divide them in 20 bins of 50 points
- Compute the bins average (pink dots)



Take the variance of the pink points and you have a sensitivity measure $V_{X_i}(E_{X_{\sim i}}(Y|X_i))$

- 1,000 blue points
- Divide them in 20 bins of 50 points
- Compute the bins average (pink dots)



Which factor has the highest $V_{X_i}(E_{X_{\sim i}}(Y|X_i))$

First-order sensitivity index

"first-order sensitivity index", or "main effect index"

$$S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{\mathrm{Var}(Y)}$$

First-order sensitivity index

"first-order sensitivity index", or "main effect index"

$$S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{\mathrm{Var}(Y)}$$

the expected reduction in variance that would be achieved if factor X_i could be fixed.
Why?

First-order sensitivity index

Because:

$$V_{X_i}(E_{X_{\sim i}}(Y|X_i)) + E_{X_i}(V_{X_{\sim i}}(Y|X_i)) = \mathrm{Var}(Y)$$

the expected reduction in variance that would be achieved if factor X_i could be fixed.

Law of Total Variance - Try to prove this!!!

First-order sensitivity index

Because:

$$V_{X_i}(E_{X_{\sim i}}(Y|X_i)) + E_{X_i}(V_{X_{\sim i}}(Y|X_i)) = \mathrm{Var}(Y)$$

This is what variance would be left (on average) if X_i could be fixed.

For additive models we can decompose the total variance as a sum of first order effects

Higher-order sensitivity index

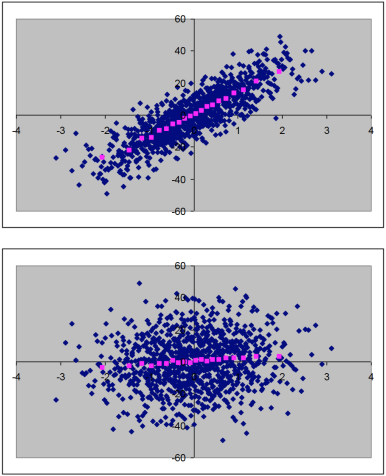
From Variance Decomposition (ANOVA):

$$V_{X_i}(E_{X_{\sim i}}(Y|X_i)) = V_i$$

$$V_{X_iX_j}(E_{X_{\sim ij}}(Y|X_iX_j)) = V_i + V_j + V_{ij}$$

Non-additive model

- Look at the second plot: Is $S_i = 0$?
- Is this factor non-important?



Total effect Sensitivity Index

$$S_{Ti} = \frac{E_{\mathbf{X}_{\sim i}}\left(\mathrm{Var}_{X_i}(Y \mid \mathbf{X}_{\sim i})\right)}{\mathrm{Var}(Y)} = 1 - \frac{\mathrm{Var}_{\mathbf{X}_{\sim i}}\left(E_{X_i}(Y \mid \mathbf{X}_{\sim i})\right)}{\mathrm{Var}(Y)}$$

the expected variance that would be left if all factors but X_i could be fixed.

Total effect Sensitivity Index

$$\sum_{i=1}^{d} S_{Ti} \geq 1$$

due to the fact that the interaction effect between e.g. X_i and X_j is counted in both S_{Ti} and S_{Tj} In fact, the sum of the S_{Ti} will only be equal to 1 when the model is purely additive.

Interpret Sensitivity Index

$$S_i = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{\mathrm{Var}(Y)}$$

Factors prioritization -If the cost of discovering factors were the same for all factors which factor should I try to discover first?

Saltelli A. Tarantola S., 2002, On the relative importance of input factors in mathematical models: safety assessment for nuclear waste disposal, Journal of American Statistical Association, 97 (459), 02-709.

Interpret Sensitivity Index

$$S_{Ti} = \frac{E_{\mathbf{X}_{\sim i}}\left(\mathrm{Var}_{X_i}(Y \mid \mathbf{X}_{\sim i})\right)}{\mathrm{Var}(Y)}$$

Fixing (dropping) non important factors - Can I fix a factor [or a subset of input factors] at any given value over their range of uncertainty without reducing significantly the output? Factor fixing is useful to achieve model simplification and relevance.

Saltelli A. Tarantola S., 2002, On the relative importance of input factors in mathematical models: safety assessment for nuclear waste disposal, Journal of American Statistical Association, 97 (459), 02-709.

Interpret Sensitivity Index

Thus given a model $Y = f(X_1, X_2, X_3)$

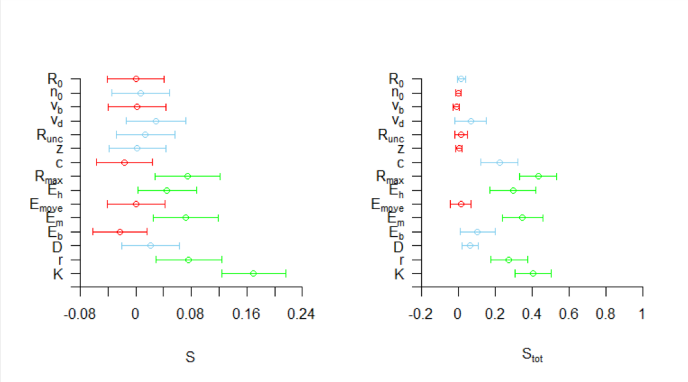
$$S_1 + S_2 + S_3 + +S_{12} + S_{13} + S_{23} + +S_{123} = 1$$

$$S_{T1} = S_1 + S_{12} + S_{13} + S_{123}$$

Dependent input parameters

- For the Sobol decomposition to hold, it is assumed that the input parameters are independent
- Many models contain correlations or other dependencies between input parameters
- In such cases, the Sobol method is **not applicable**
- For our present test-case, all parameters were sampled from independent uniform probability densities

Results of Sobol' method



- Left graph: excludes interaction effects; Right graph: includes all interaction effects
- K is influential; Observe c

Summary: Steps for Sobol method

- What output variables and input parameters (preferably all) to include
- Assign probability densities to each parameter
- Generate random input samples
- Run the model for each sample, and store outputs
- Compute first- and total-order sensitivity indices

Other Methods

Density based
VARS (Variogram Analysis of Response Surfaces)
PCE (Polynomial Chaos Expansion)
Morris

Law of total variance

Derivation of the law of total variance

$$\boxed{\text{var}(X) = \mathbf{E}\big[\text{var}(X \mid Y)\big] + \text{var}\big(\mathbf{E}[X \mid Y]\big)}$$

- $\text{var}(X) = \mathbf{E}[X^2] - (\mathbf{E}[X])^2$

$$\text{var}(X \mid Y = y) = E[X^2 \mid Y=y] - (E[X \mid Y=y])^2 \quad \text{for all } y$$

$$\text{var}(X \mid Y) = E[X^2 \mid Y] - (E[X \mid Y])^2$$

$$\mathbf{E}\big[\text{var}(X \mid Y)\big] = E[X^2] - \cancel{E\big[(E[X \mid Y])^2\big]}$$

$+$

$$\text{var}\big(\mathbf{E}[X \mid Y]\big) = E\big[\cancel{(E[X \mid Y])^2}\big] - \big(E[E[X \mid Y]]\big)^2$$

$$(E[X])^2$$

References I

- Slides Adapted from Global Sensitivity Analysis by Eugene Kirpichov (Google)
- Sensitivity Analysis @andreasaltelli, Centre for the Study of the Sciences and the Humanities, University of Bergen Presentation at Technical University of Denmark - DTU, Lyngby Campus, Chemical Engineering, June 1st 2017