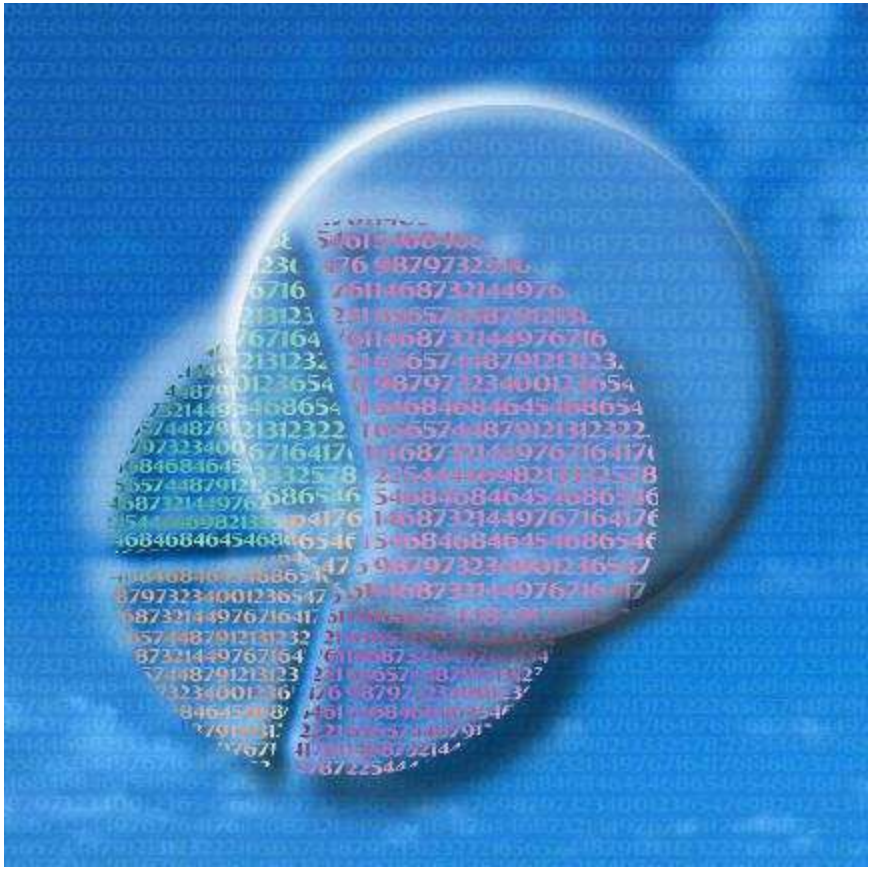

Sensitivity Analysis

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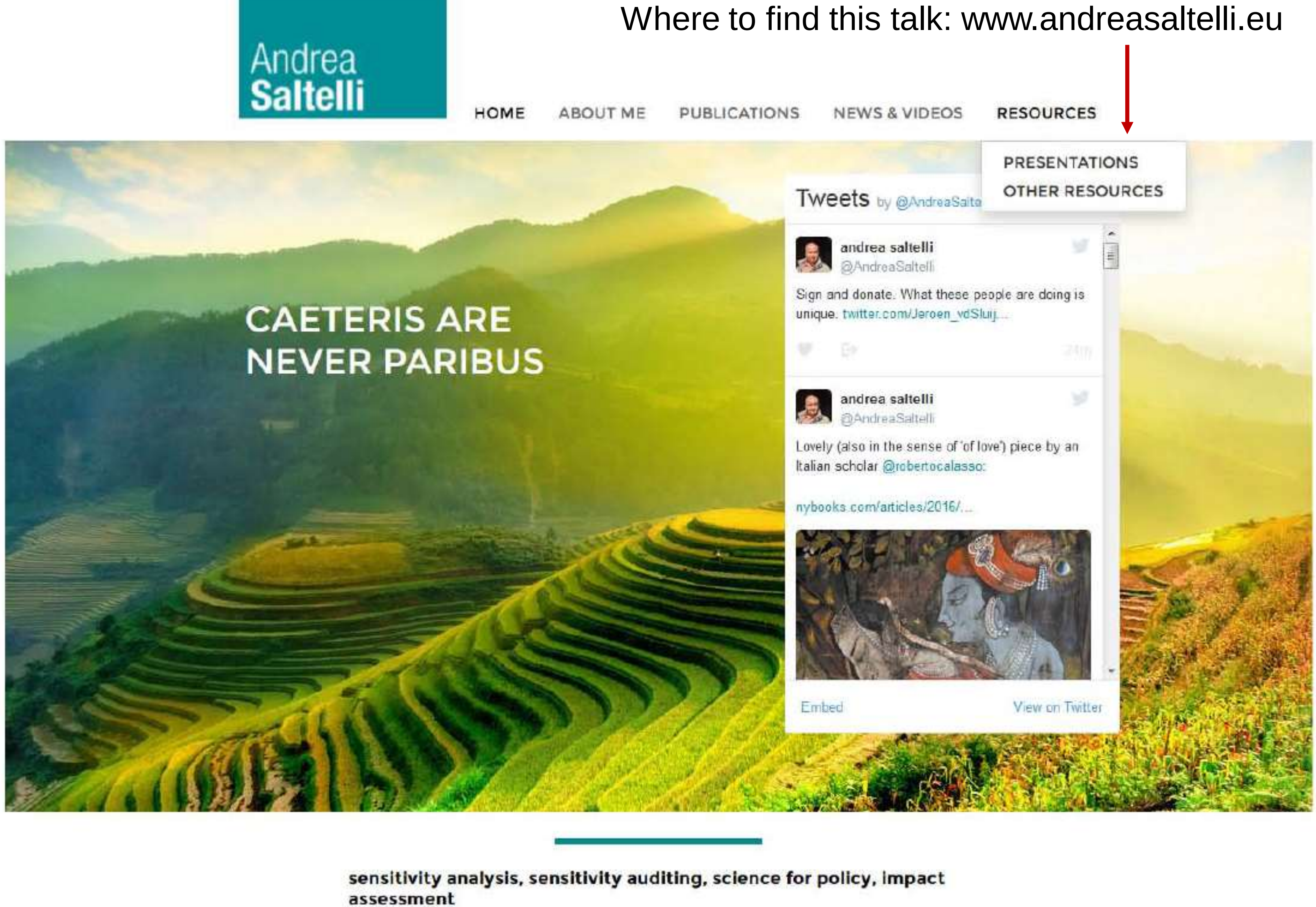
PhD-course

Numbers for policy: Practical problems in quantification

Bergen, March 13-17, 2017

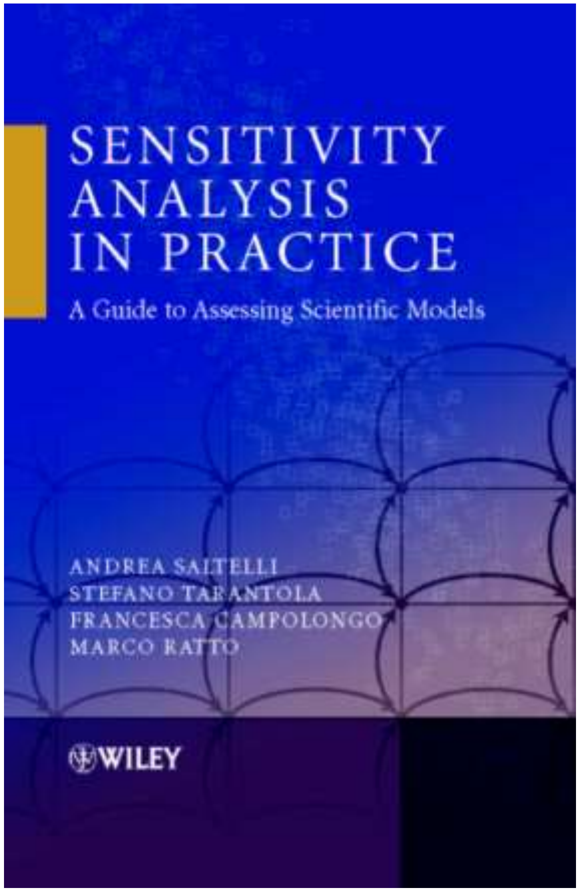
Where to find this talk: www.andreasaltelli.eu

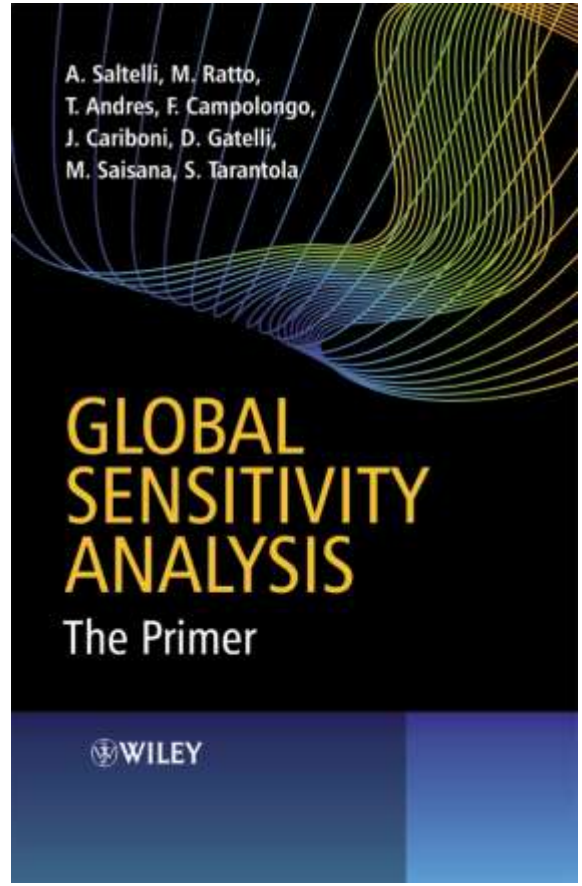


= more material on my web site

= discussion time

Sensitivity analysis books available on LibGen





What is sensitivity analysis?

Definitions

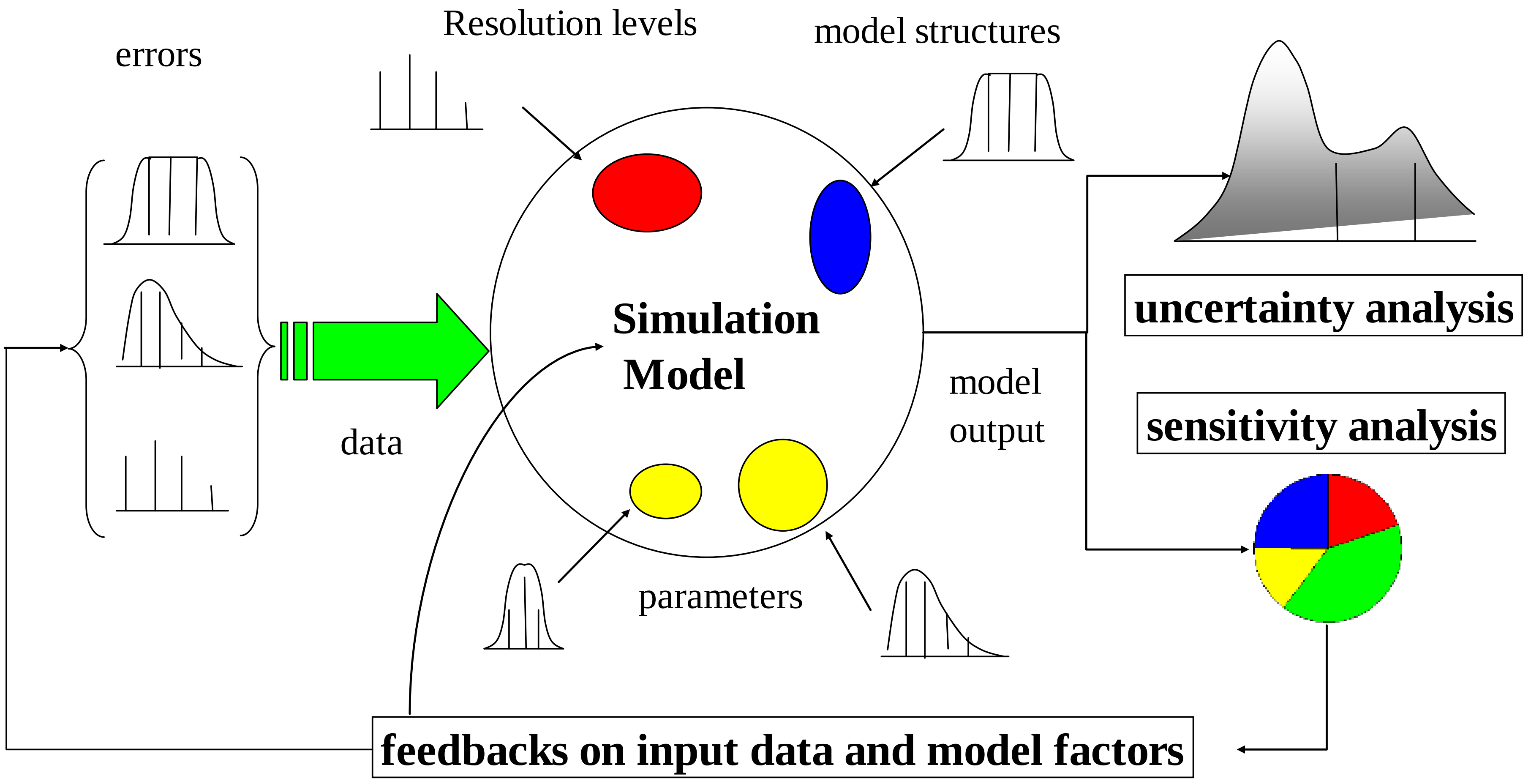
Uncertainty analysis: Focuses on just quantifying the uncertainty in model output

Sensitivity analysis: The study of the relative importance of different input factors on the model output

[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.

An engineer's vision of UA, SA



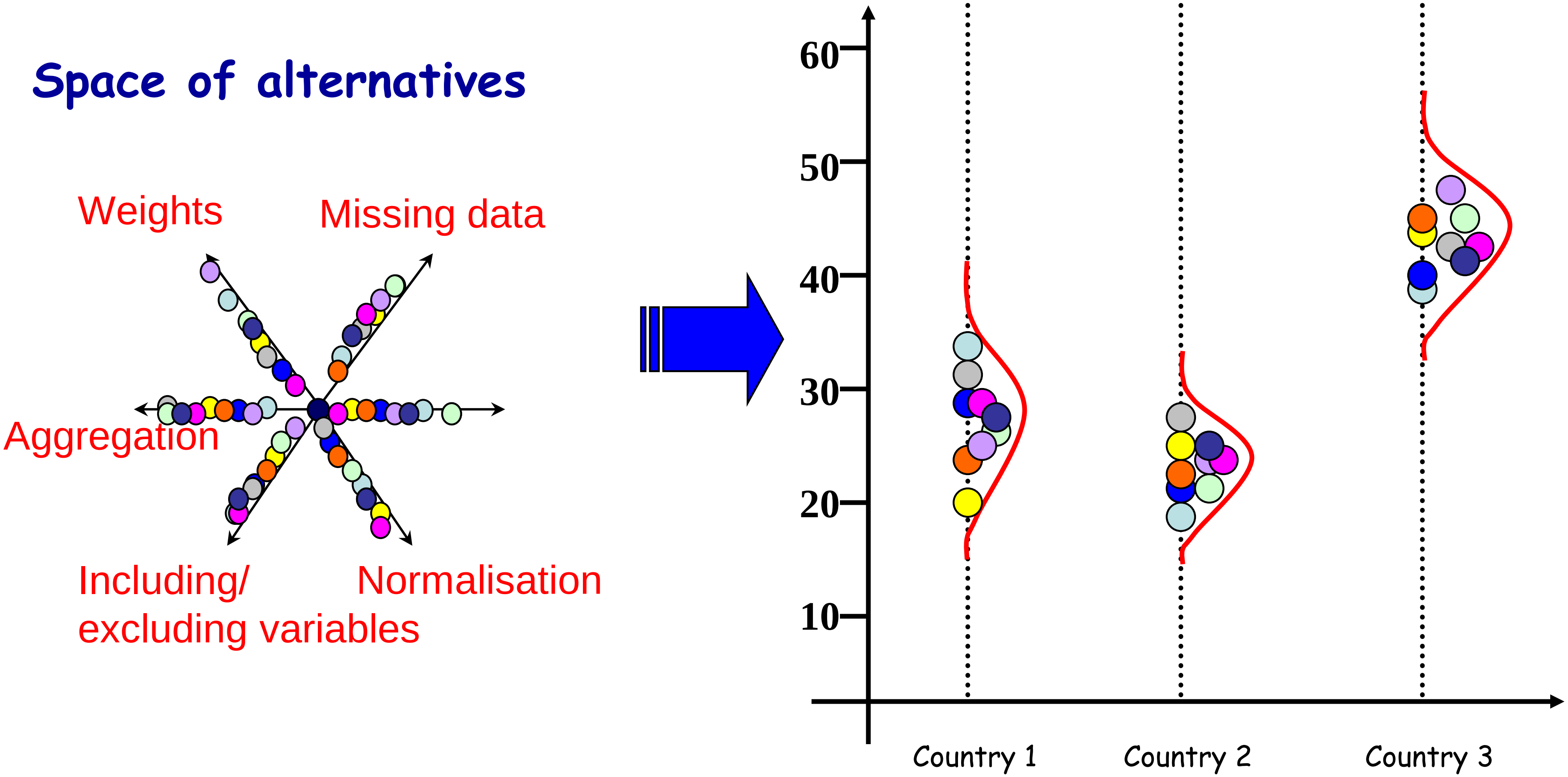
One can sample more than just factors

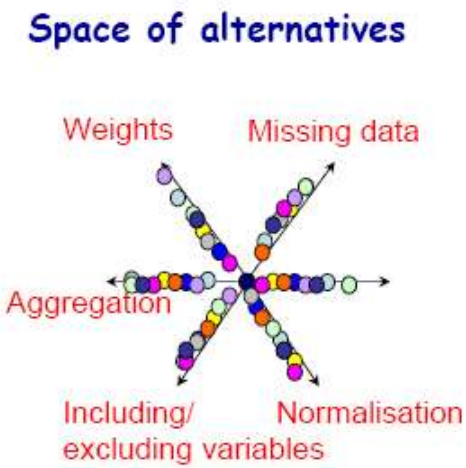
One can sample modelling assumptions

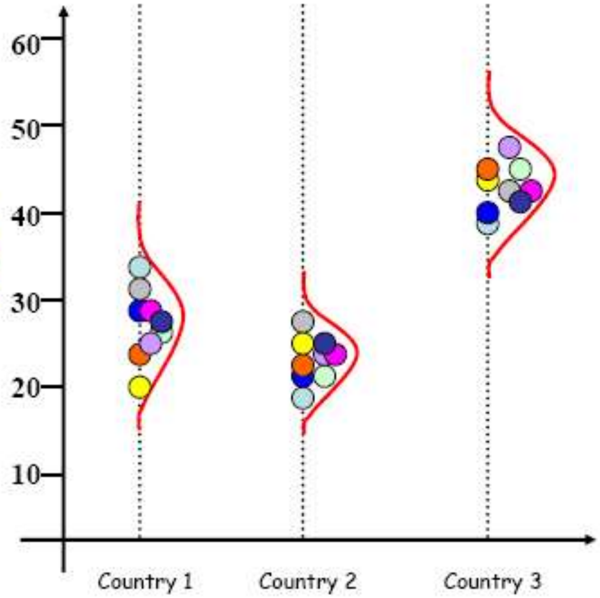
Example: The output is a composite indicator

Assumption	Alternatives
Number of indicators	▪ all six indicators included or one-at-time excluded (6 options)
Weighting method	▪ original set of weights, ▪ factor analysis, ▪ equal weighting, ▪ data envelopment analysis
Aggregation rule	▪ additive, ▪ multiplicative, ▪ Borda multi-criterion

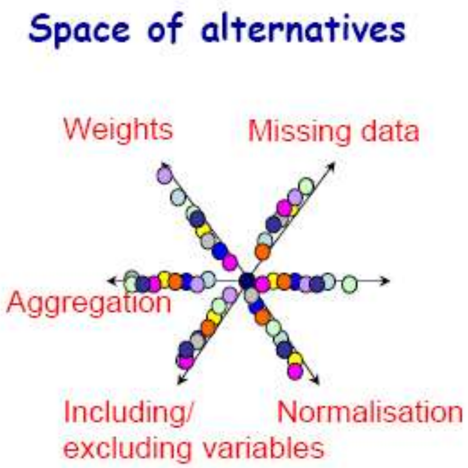
Space of alternatives

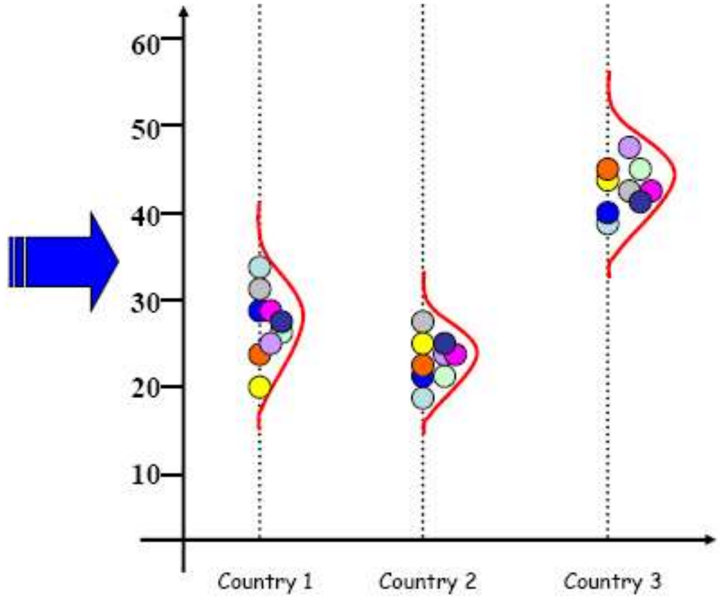






Is this an uncertainty analysis or a sensitivity analysis?





If I did a sensitivity analysis what information would I obtain?

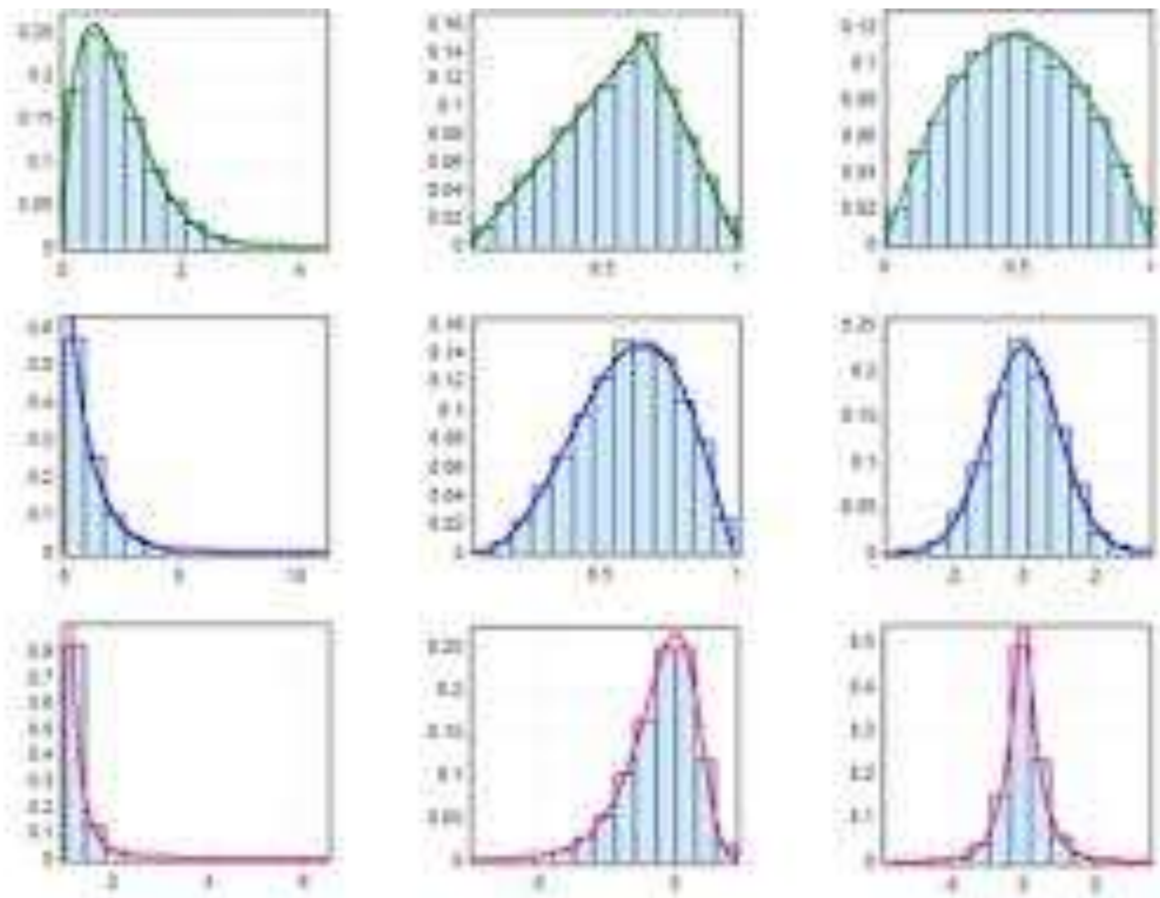
Sample matrix for uncertainty and sensitivity analysis

$$
\begin{matrix}
x_{11} & x_{12} & \cdots & x_{1k} \\
x_{21} & x_{22} & \cdots & x_{2k} \\
\cdots & \cdots & \cdots & \cdots \\
x_{N1} & x_{N2} & \cdots & x_{Nk}
\end{matrix}
$$

Each row is a sample trial for one model run. Each column is a sample of size N from the distribution of the factor.

Each column is a sample of size N from the distribution of factor.

$$\begin{matrix} x_{11} & x_{12} & \dots & x_{1k} \\ x_{21} & x_{22} & \dots & x_{2k} \\ \dots & \dots & \dots & \dots \\ x_{N1} & x_{N2} & \dots & x_{Nk} \end{matrix}$$



Model results:

Each entry is the error-free result of the model run.

$$y_1$$
$$y_2$$
$$\ldots$$
$$y_N$$

$$\begin{matrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \cdots & \cdots & \cdots & \cdots \\ x_{N1} & x_{N2} & \cdots & x_{Nk} \end{matrix} \qquad \begin{matrix} y_1 \\ y_2 \\ \cdots \\ y_N \end{matrix}$$

Input matrix

Output vector:

In the simplest case y could be a function of – a simple mathematical expression of – the $x_1, x_2, \cdots x_k$

e.g. $y = x_1 \sin(x_2)/x_3$

Or it could be a more complicate mathematical model in a computer code to generate y given $x_1, x_2, \cdots x_k$

Why Sensitivity analysis?

European Commission, 2015

Office for the Management and Budget, 2006

Environmental Protection Agency, 2009

EPA, 2009, March. Guidance on the Development, Evaluation, and Application of Environmental Models. Technical Report EPA/100/K-09/003. Office of the Science Advisor, Council for Regulatory Environmental Modeling, http://nepis.epa.gov/Exe/ZyPDF.cgi?Dockey=P1003E4R.PDF, Last accessed December 2015.

EUROPEAN COMMISSION, Better regulation toolbox, appendix to the Better Regulation Guidelines, Strasbourg, 19.5.2015, SWD(2015) 111 final, COM(2015) 215 final, http://ec.europa.eu/smart-regulation/guidelines/docs/swd_br_guidelines_en.pdf.

OMB, Proposed risk assessment bulletin, Technical report, The Office of Management and Budget's – Office of Information and Regulatory Affairs (OIRA), January 2006, https://www.whitehouse.gov/sites/default/files/omb/assets/omb/inforeg/proposed_risk_assessment_bulletin_010906.pdf, pp. 16–17, accessed December 2015.

http://ec.europa.eu/smart-regulation/

Source: IA Toolbox, p. 391

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Better Regulation "Toolbox"

4. Sensitivity and uncertainty analyses

Page 391

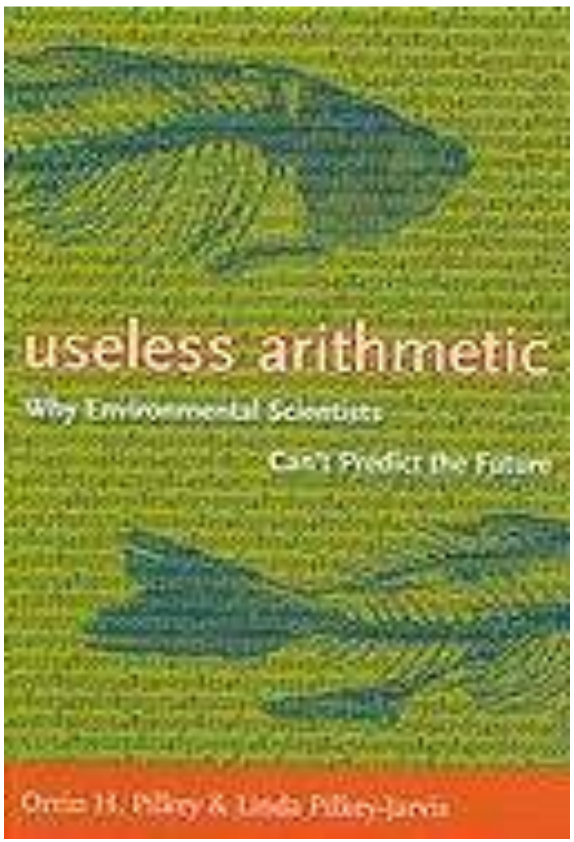
Six steps for a global SA:

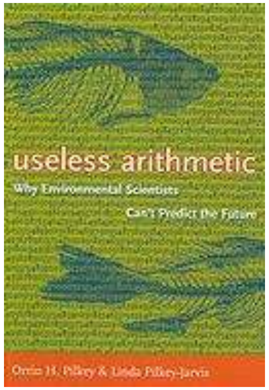
1. Select one output of interest;
2. Participatory step: discuss which input may matter;
3. Participatory step (extended peer review): define distributions;
4. Sample from the distributions;
5. Run (=evaluate) the model for the sampled values;
6. Obtain in this way bot the uncertainty of the prediction and the relative importance of variables.

Limits of sensitivity analysis

Orrin H. Pilkey
Duke University, NC

Useless Arithmetic: Why Environmental Scientists Can't Predict the Future
by Orrin H. Pilkey and Linda Pilkey-Jarvis



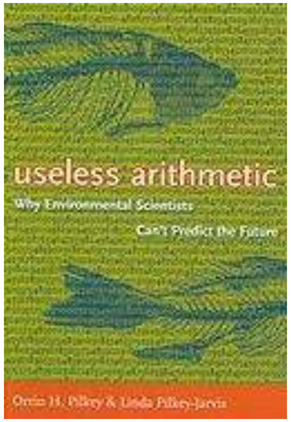


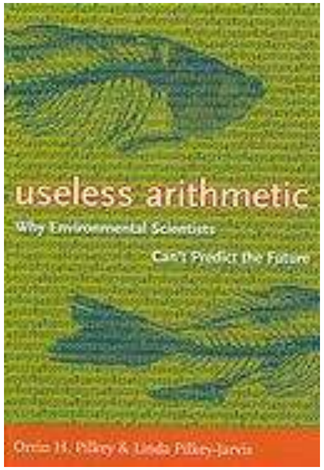
<<It is important, however, to recognize that the sensitivity of the parameter in the equation is what is being determined, not the sensitivity of the parameter in nature.

[…] If the model is wrong or if it is a poor representation of reality, determining the sensitivity of an individual parameter in the model is a meaningless pursuit.>>

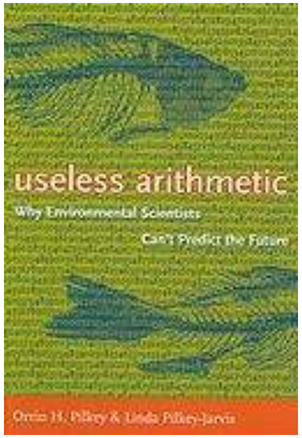
One of the examples discussed concerns the Yucca Mountain repository for radioactive waste. TSPA model (for total system performance assessment) for safety analysis.

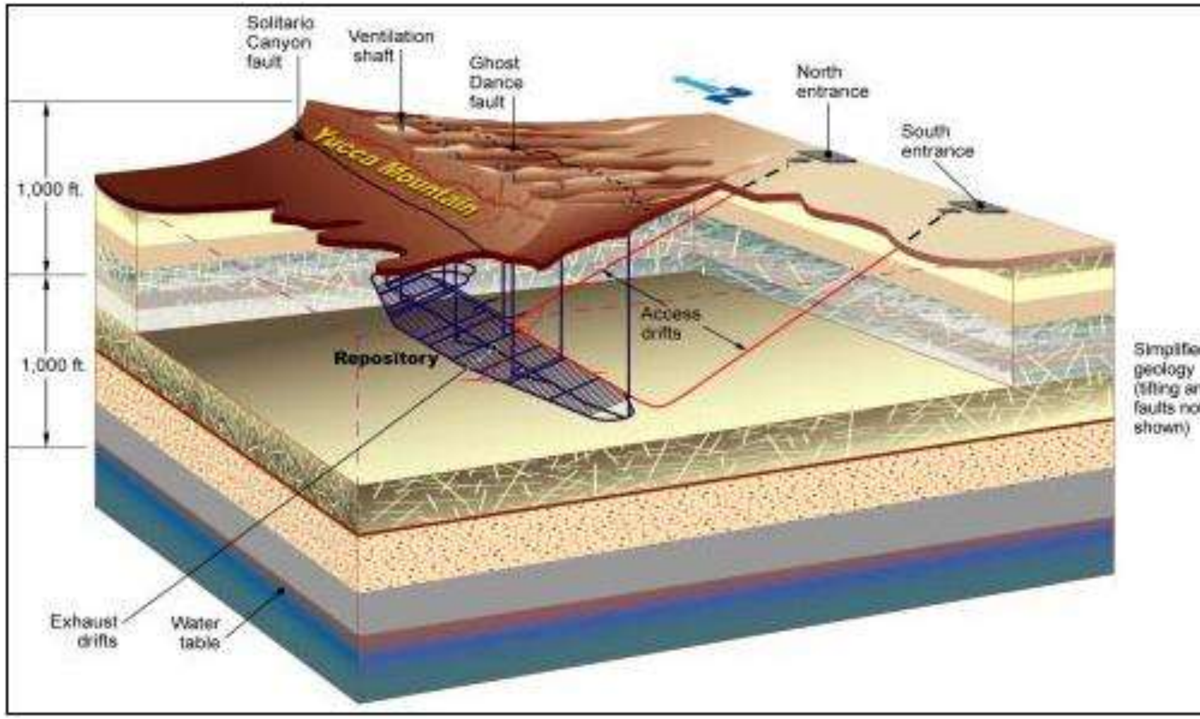
TSPA is Composed of 286 sub-models.





TSPA (like any other model) relies on assumptions → one is the low permeability of the geological formation → long time for the water to percolate from surface to disposal.





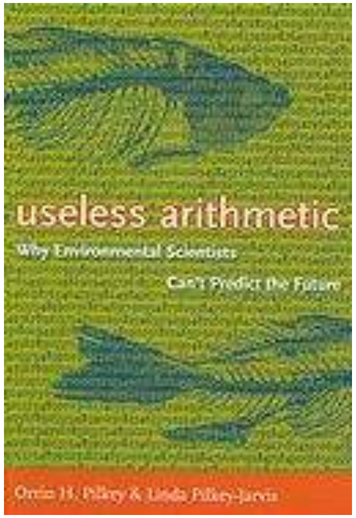
The confidence of the stakeholders in TSPA was not helped when evidence was produced which could lead to an upward revision of 4 orders of magnitude of this parameter

(the ^{36}Cl story)

Type III error in sensitivity: Examples:

In the case of TSPA (Yucca mountain) a range of 0.02 to 1 millimetre per year was used for percolation of flux rate.

→… SA useless if it is instead ~ 3,000 millimetres per year.



"Scientific mathematical modelling should involve constant efforts to falsify the model"

Ref. ➔ Robert K. Merton's 'Organized skepticism '

Robert K. Merton

Communalism – the common ownership of scient40

ific discoveries, according to which scientists give up intellectual property rights in exchange for recognition and esteem (Merton actually used the term Communism, but had this notion of communalism in mind, not Marxism);

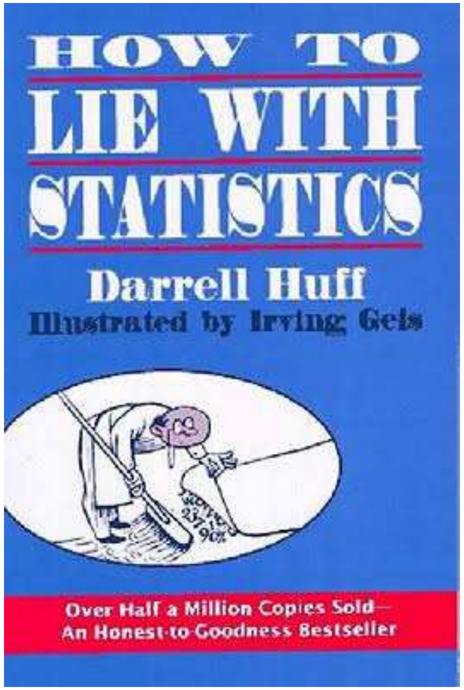
Universalism – according to which claims to truth are evaluated in terms of universal or impersonal criteria, and not on the basis of race, class, gender, religion, or nationality;

Disinterestedness – according to which scientists are rewarded for acting in ways that outwardly appear to be selfless;

Organized Skepticism – all ideas must be tested and are subject to rigorous, structured community scrutiny.

Can I lie with sensitivity analysis?

Will any sensitivity analysis do the job? Can I lie with sensitivity analysis as I can lie with statistics?



Saltelli, A., Annoni P., 2010, How to avoid a perfunctory sensitivity analysis, *Environmental Modeling and Software,* **25**, 1508–1517.

Why not just changing one factor at a time (OAT)?

<<"one-at-a-time" (OAT) approach is most commonly used in Commission IAs>>

Source: IA Toolbox, p. 391

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Why not just changing one factor at a time (OAT)?

"Sensitivity analysis usually proceeds by changing one variable or assumption at a time, but it can also be done by varying a combination of variables simultaneously to learn more about the robustness of your results to widespread changes".

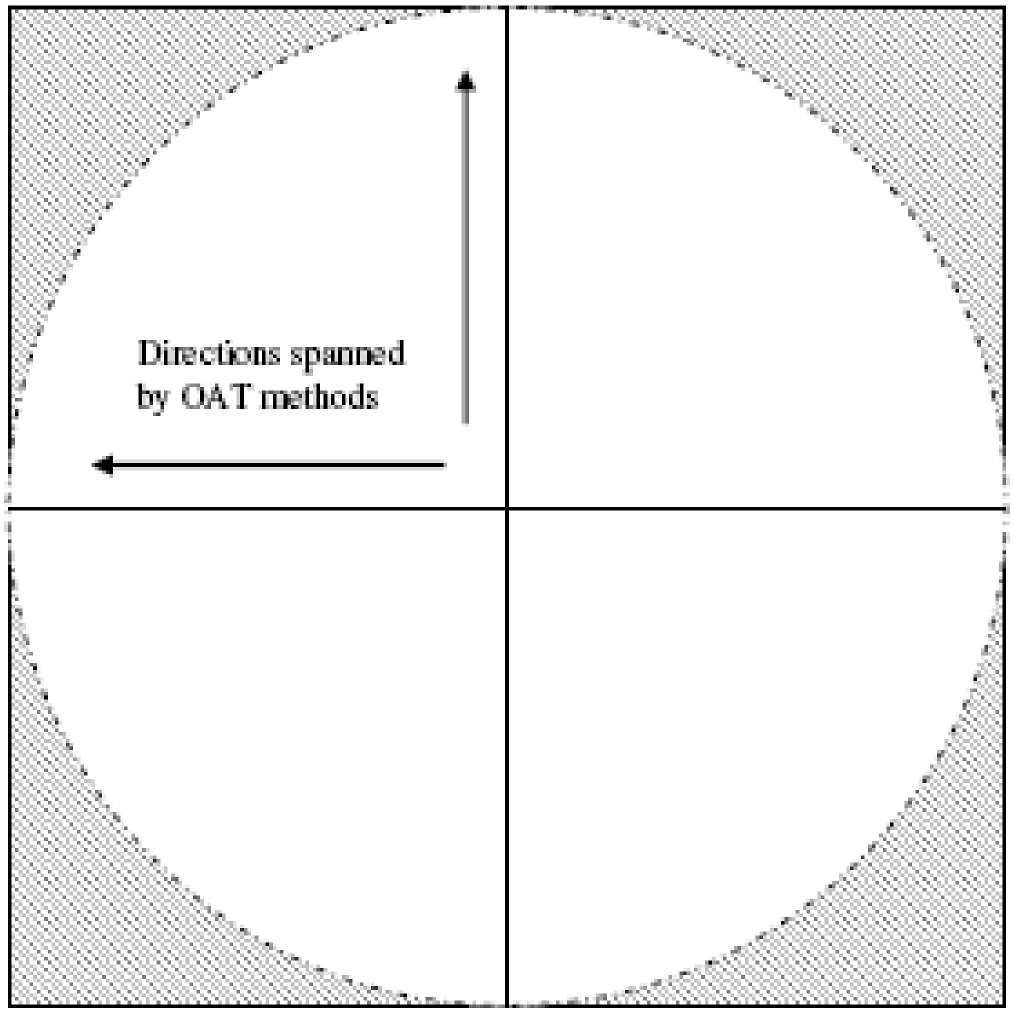
Source: Office for the management and Budget of the White House (OMB), Circular A4, 2003

https://www.whitehouse.gov/omb/circulars_a004_a-4/

Why not just changing one factor at a time (OAT)?

Because it is a bad idea!

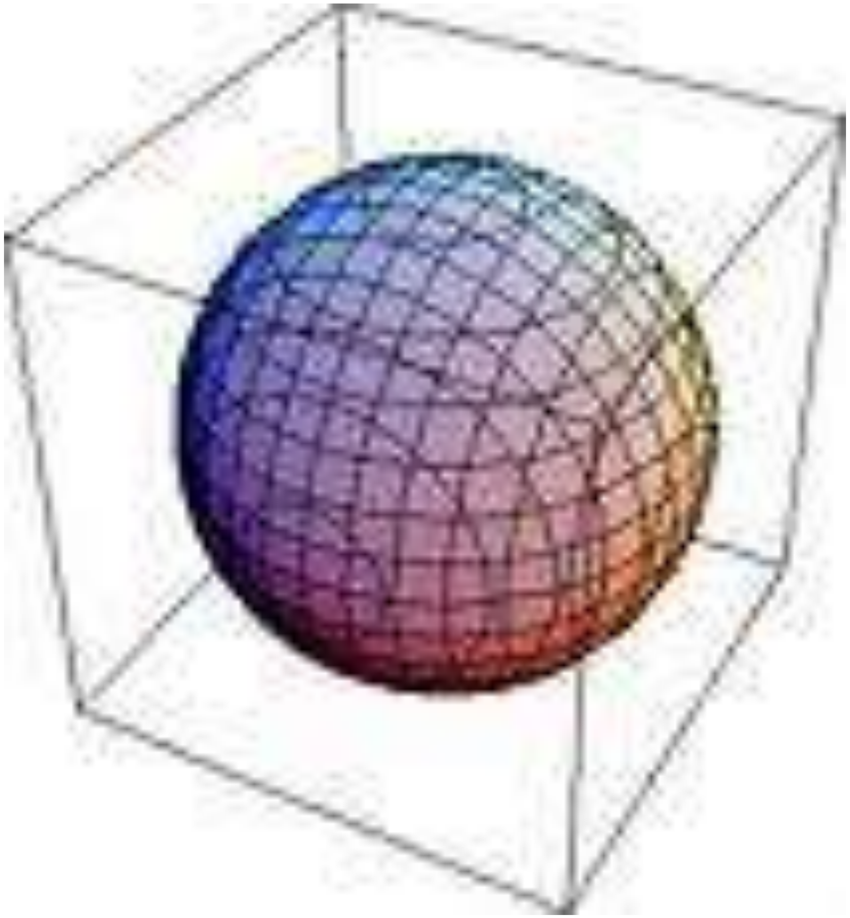
OAT in 2 dimensions



Area circle / area square =?

~ 3/4

OAT in 3 dimensions



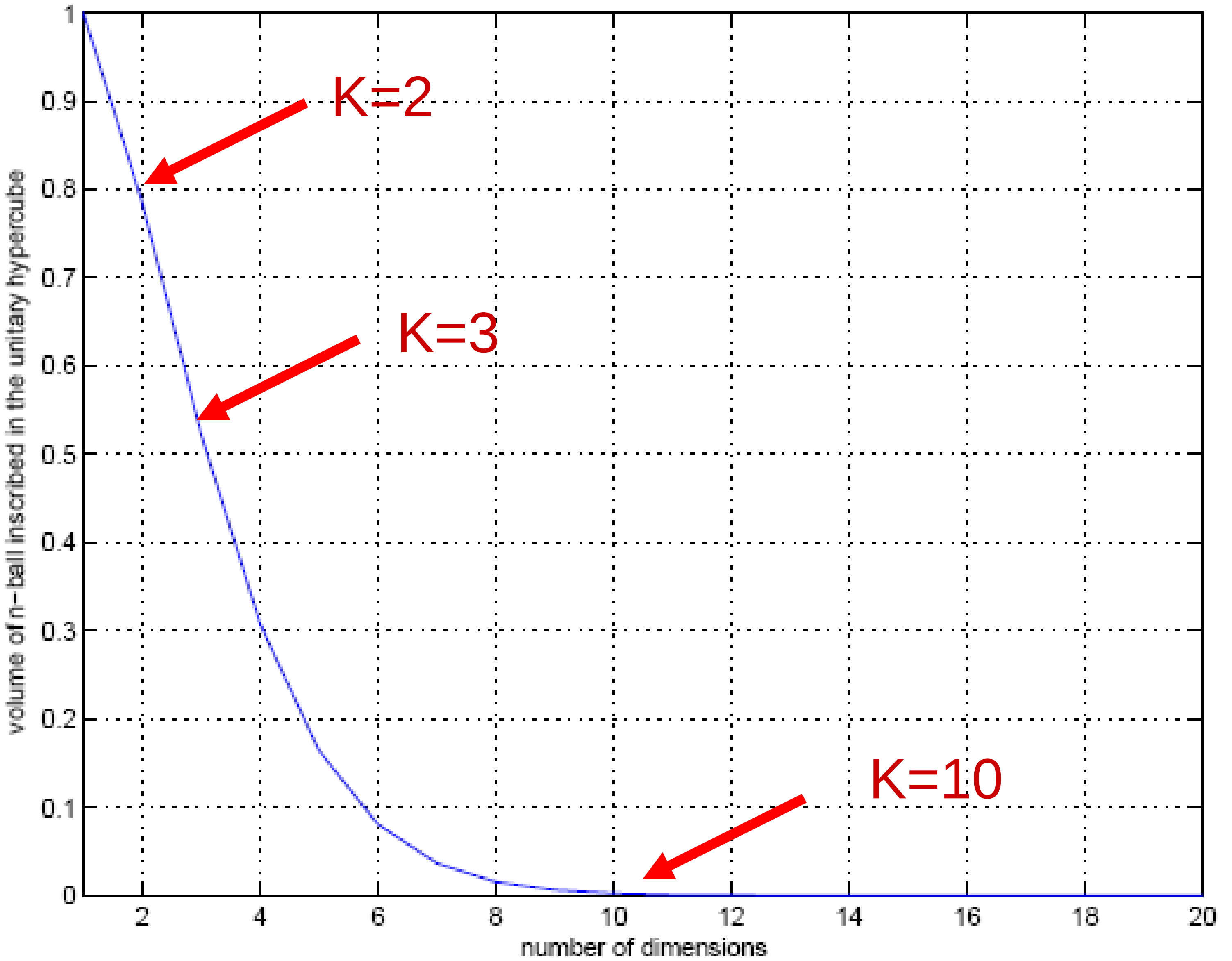
Volume sphere / volume cube =?

~ 1/2

OAT in 10 dimensions

Volume hypersphere / volume ten dimensional hypercube ~ 0.0025

OAT in k dimensions

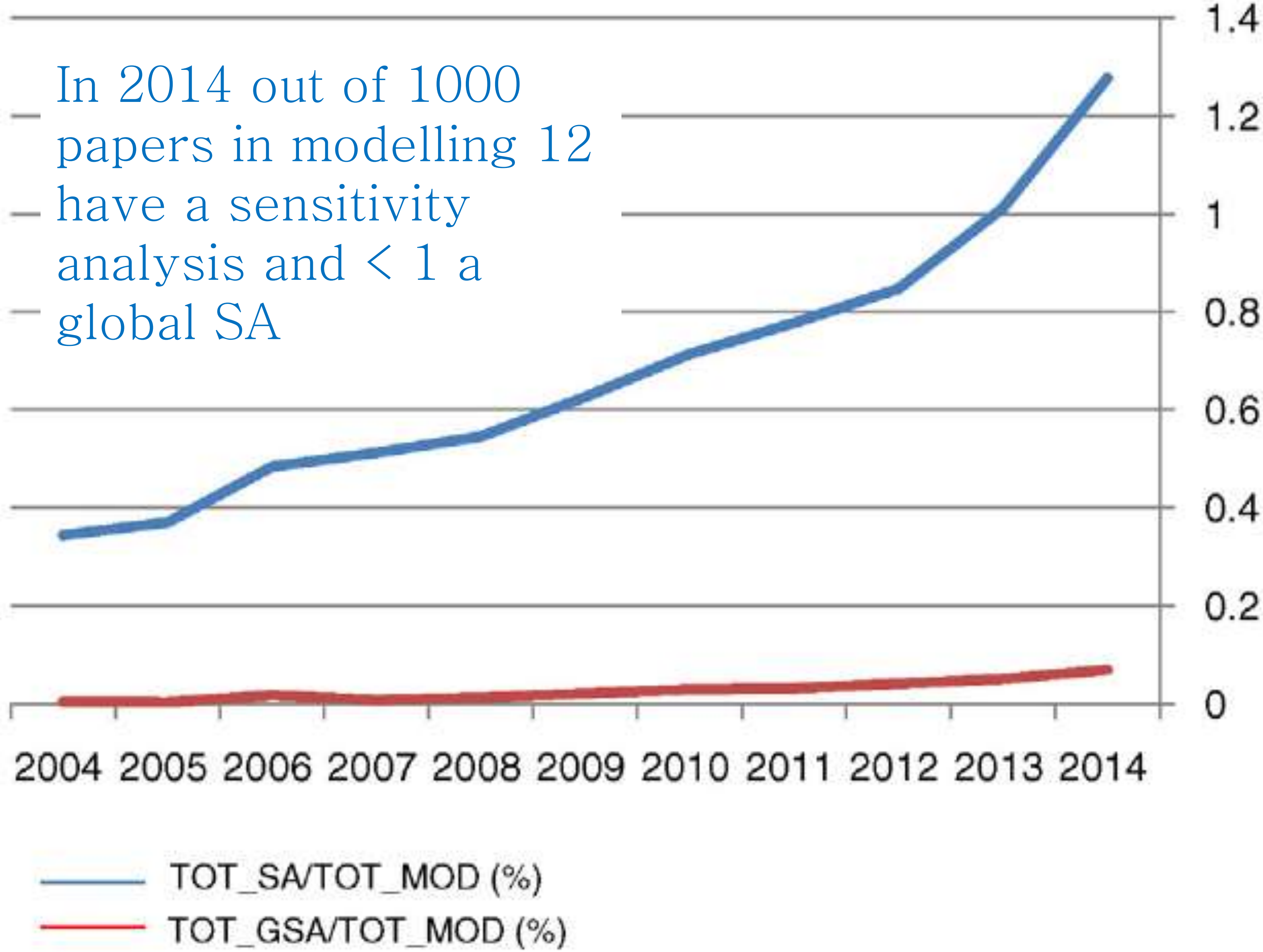


Bottom-line: once a sensitivity analysis is done via OAT there is no guarantee that either uncertainty analysis (UA) or sensitivity analysis (SA) is any good:

- ➔ UA will be non conservative
- ➔ SA may miss important factors

OAT is still the most largely used technique in SA. Out of every 100 papers with modelling & SA only 4 are ‘global’ in the sense discussed here.

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


In 2014 out of 1000 papers in modelling 12 have a sensitivity analysis and < 1 a global SA
1.4
1.2
1
0.8
0.6
0.4
0.2
0
2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014
TOT_SA/TOT_MOD (%)
TOT_GSA/TOT_MOD (%)

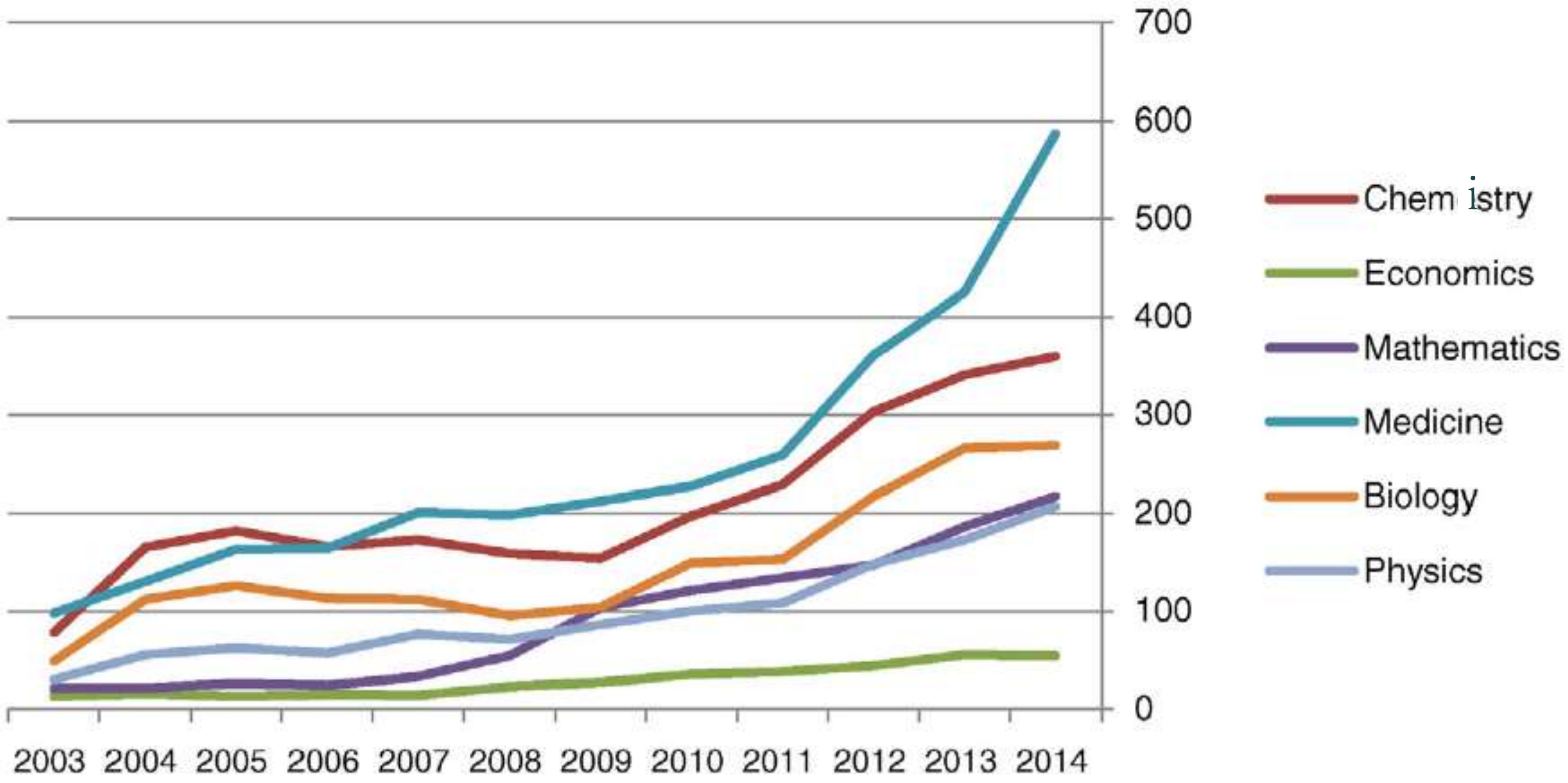


Fig. 4. GSA in the different scientific domains.

Discussion points (1)

- Is the geometric argument necessary? Anyone experience in design of experiment (DOE)?
- Can OAT be justified in some cases?

Discussion points (2)

The influence of the key variables should be investigated by a sensitivity analysis.

- Is something wrong about the statement above (p. 384 of EC guidelines)

Discussion points (3)

- If I keep a parameter fixed I am in error, if I give it a distribution there are problems to justify it … is this a law of constant misery?

How is sensitivity analysis done?

$$\begin{matrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \cdots & \cdots & \cdots & \cdots \\ x_{N1} & x_{N2} & \cdots & x_{Nk} \end{matrix}$$

Input matrix

$$\begin{matrix} y_1 \\ y_2 \\ \cdots \\ y_N \end{matrix}$$

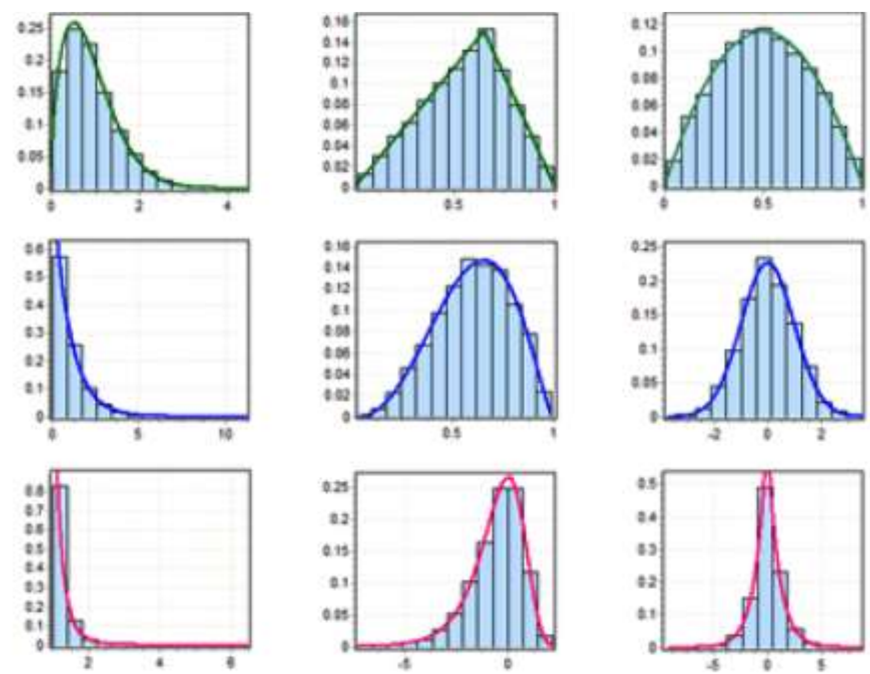
Output vector:

$$
\begin{matrix}
x_{11} & x_{12} & \cdots & x_{1k} \\
x_{21} & x_{22} & \cdots & x_{2k} \\
\cdots & \cdots & \cdots & \cdots \\
x_{N1} & x_{N2} & \cdots & x_{Nk}
\end{matrix}
$$

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



Examples of distributions of input factors

$$
\begin{array}{ccccc}
x_{11} & x_{12} & \cdots & x_{1k} & \longrightarrow & y_1 \\
x_{21} & x_{22} & \cdots & x_{2k} & \longrightarrow & y_2 \\
\cdots & \cdots & \cdots & \cdots & & \cdots \\
x_{N1} & x_{N2} & \cdots & x_{Nk} & \longrightarrow & y_N
\end{array}
$$

Output vector:

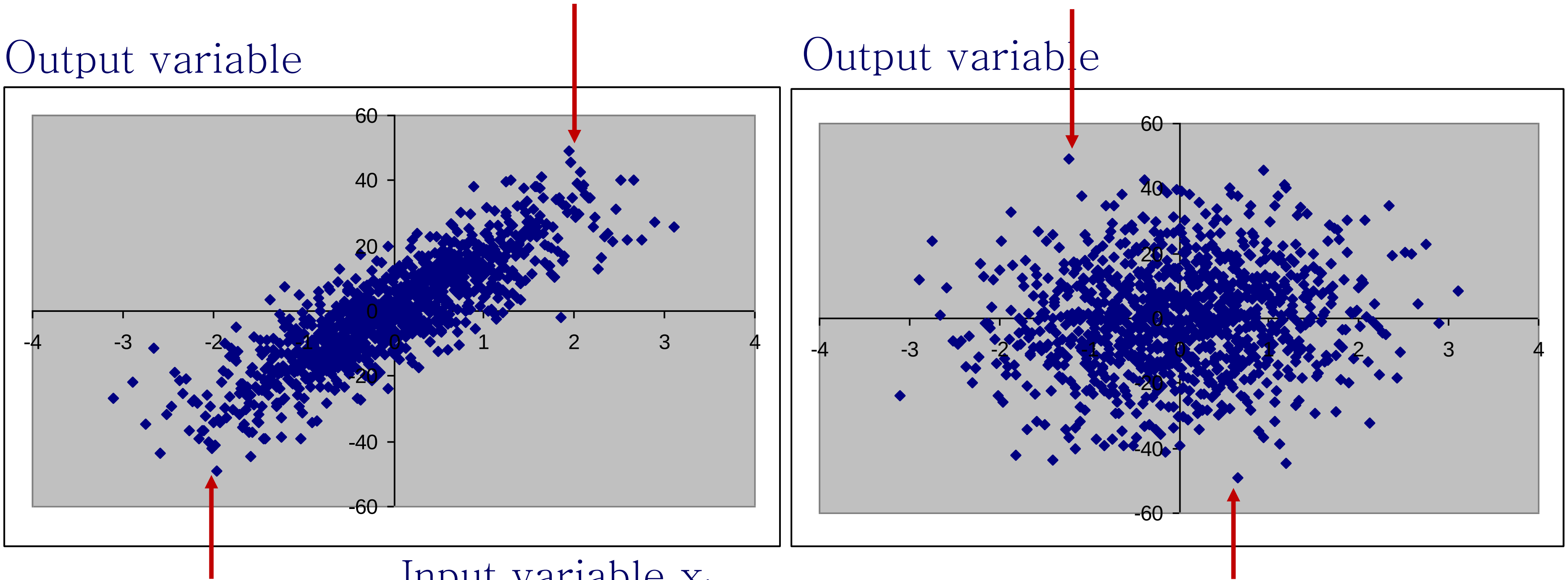
- Just one output of interest; but y could also be a vector (function of time) or a map, etc. …

- Y can be plotted against any of the x_i

Y plotted against two different factors x_i and x_j

Output variable

Output variable

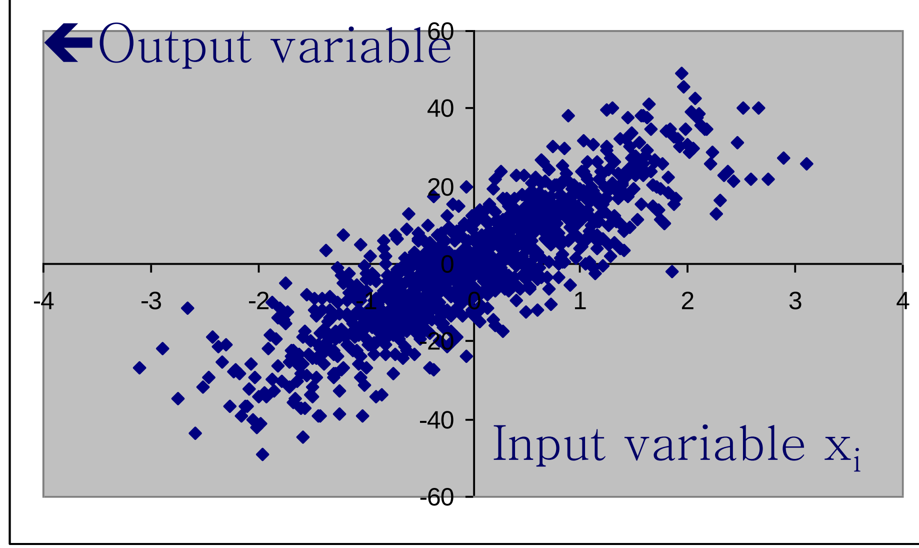


Input variable x_i

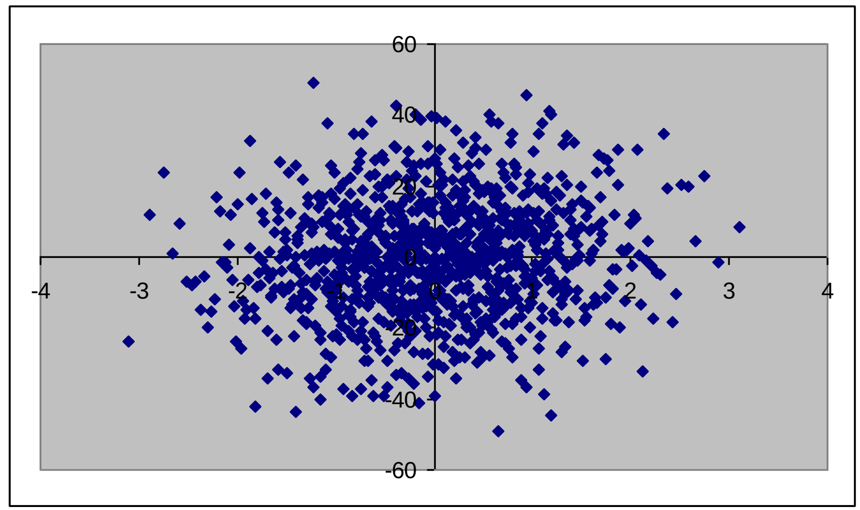
Input variable x_j

The values of the output on the ordinate are the same

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

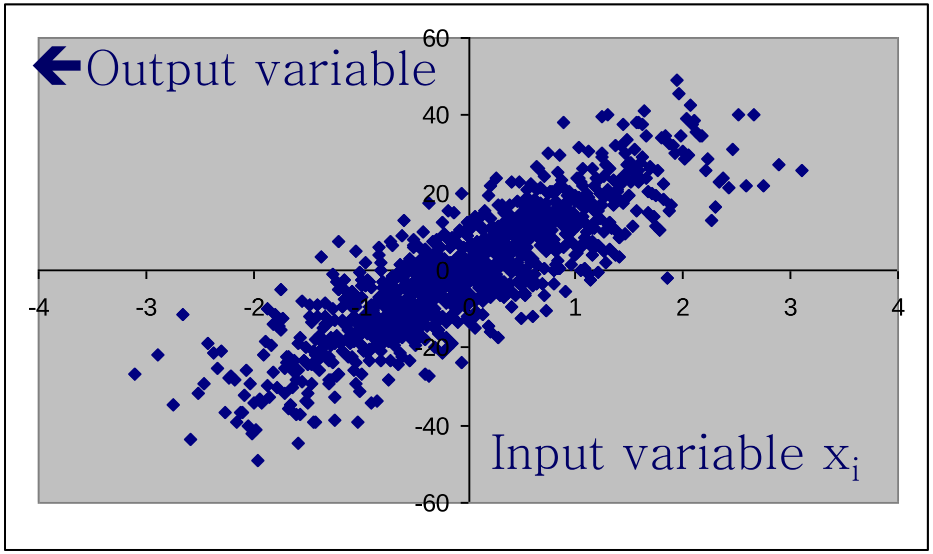


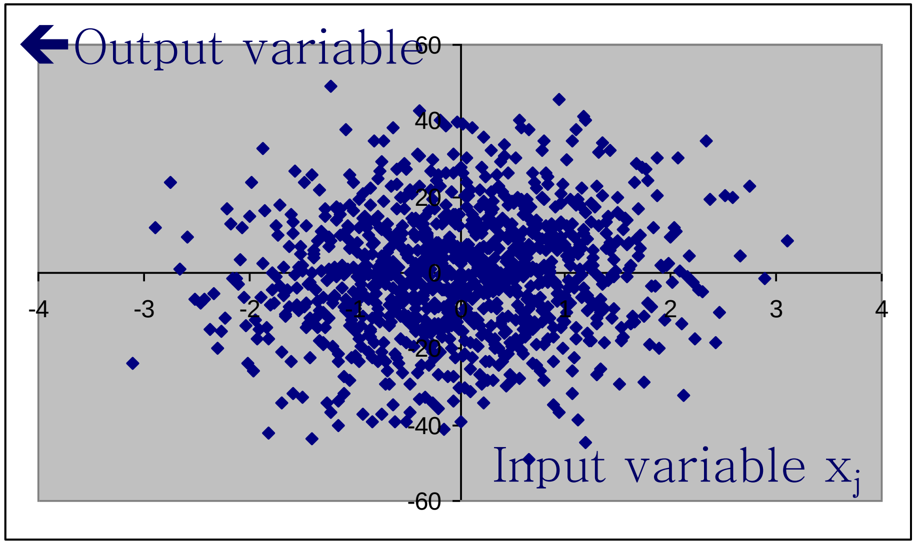
Output variable →



Input variable x_j

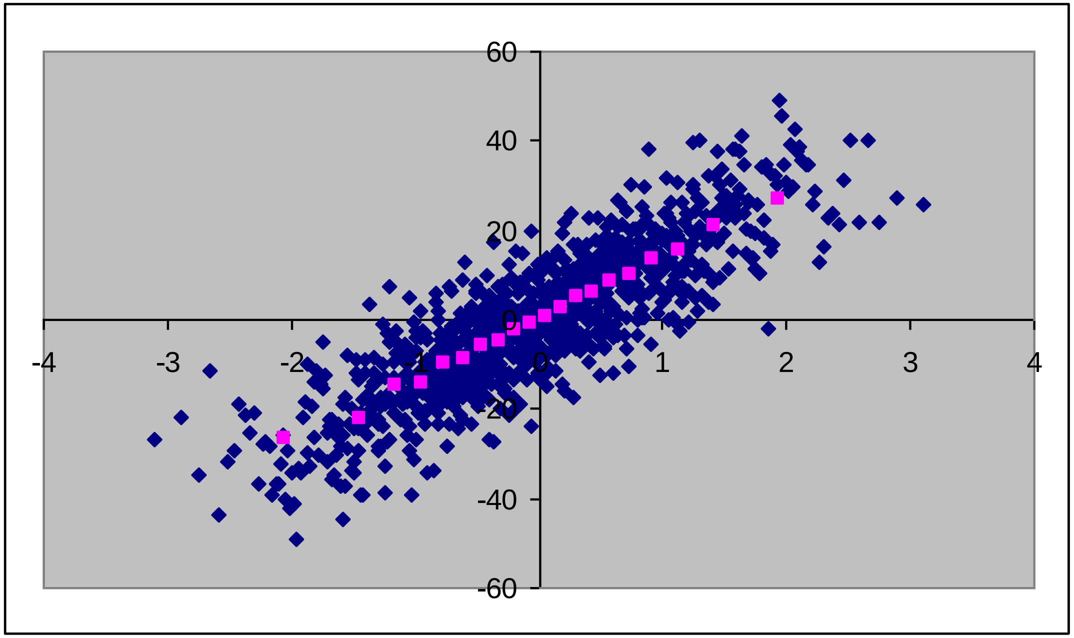
Scatterplots of y versus sorted factors

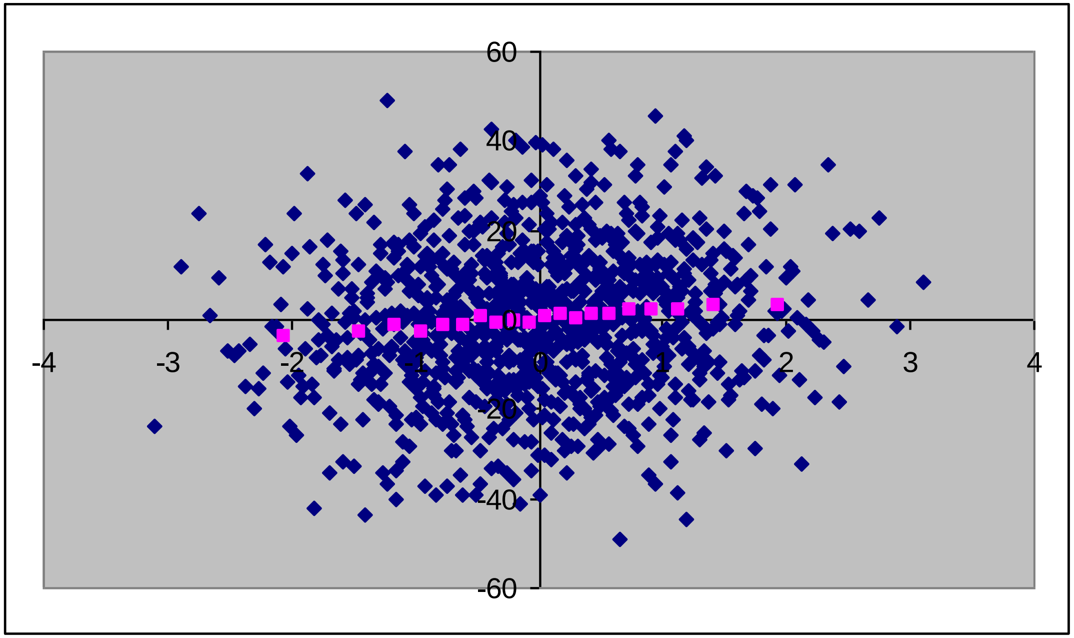




Which factor is more important?

Why?

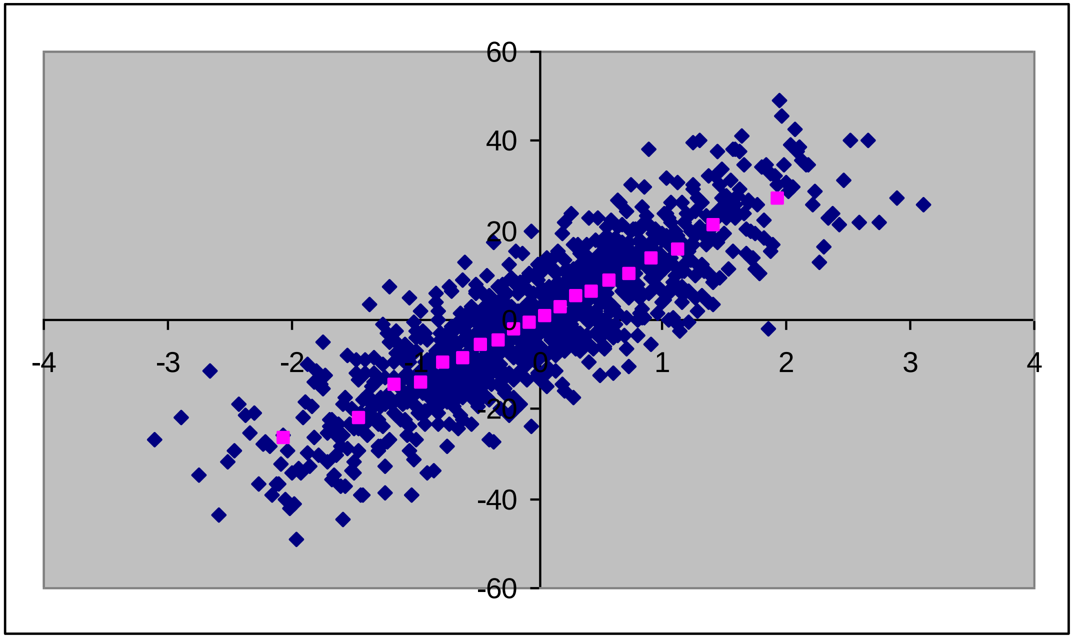




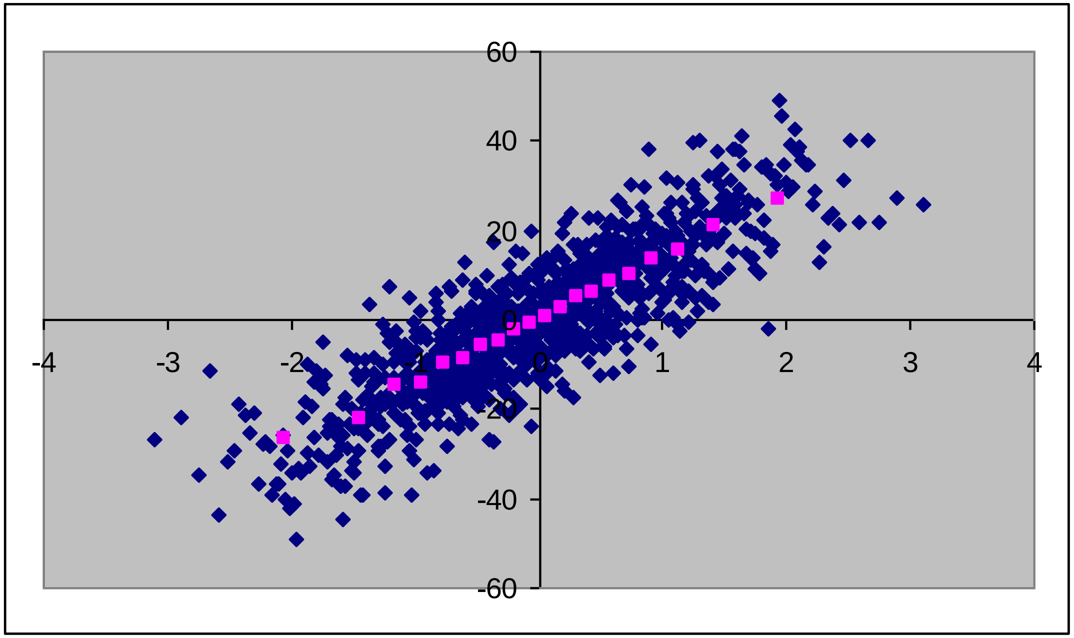
~1,000 blue points

Divide them in 20 bins of ~ 50 points

Compute the bin's average (pink dots)

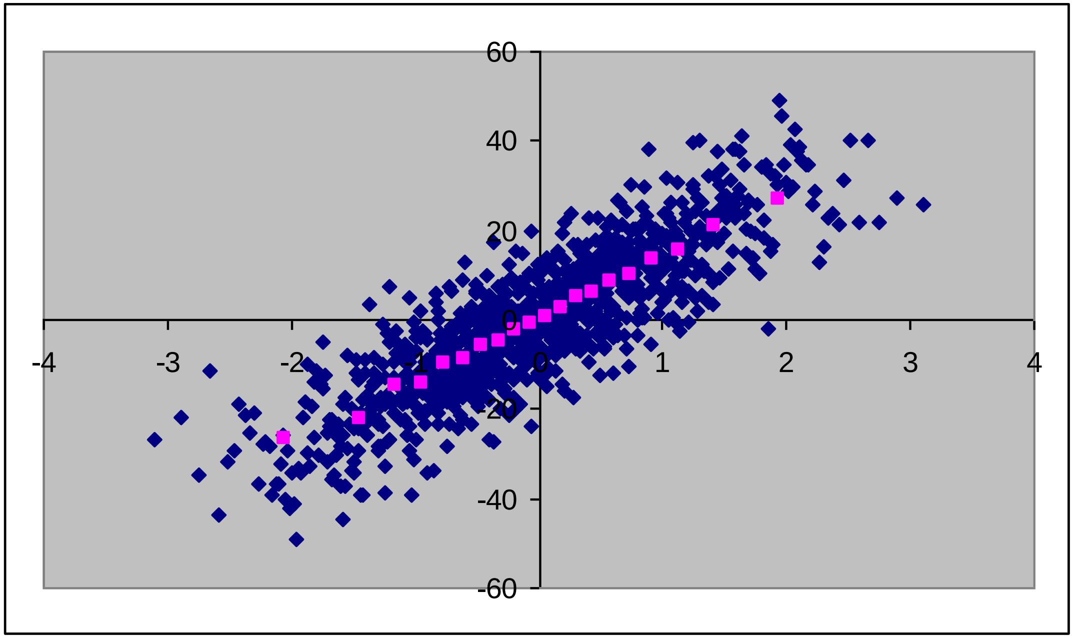


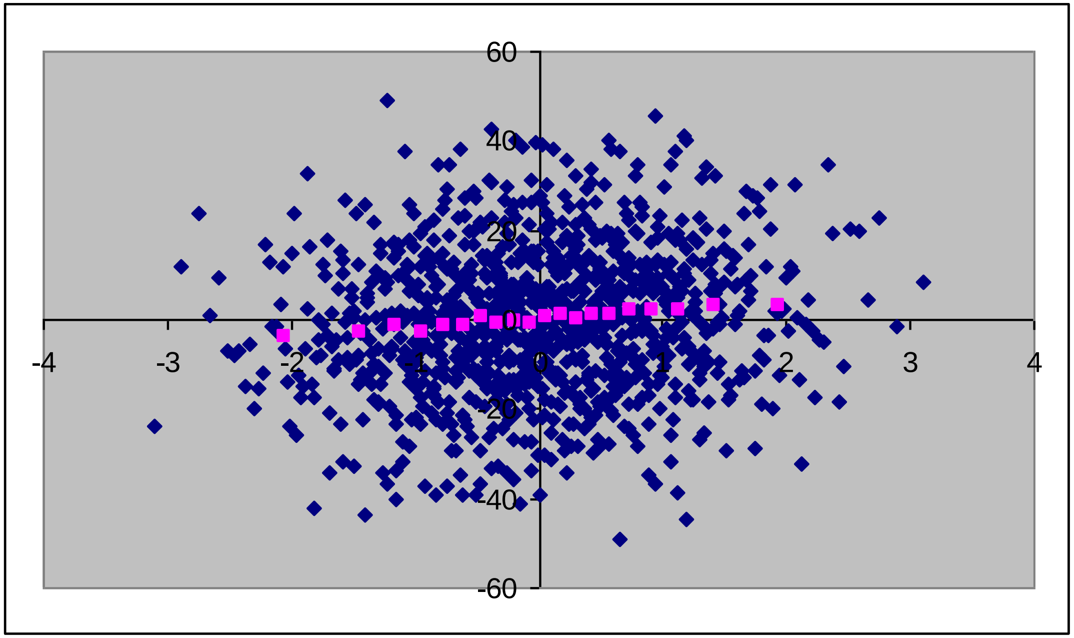
Each pink point is ~ $E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)$



Take the variance of the pink points and you have a sensitivity measure

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right)$$





Which factor has the highest $V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y|X_i\right)\right)$?

$$S_i \equiv \frac{V\left(E\left(Y \middle| X_i\right)\right)}{V_Y}$$

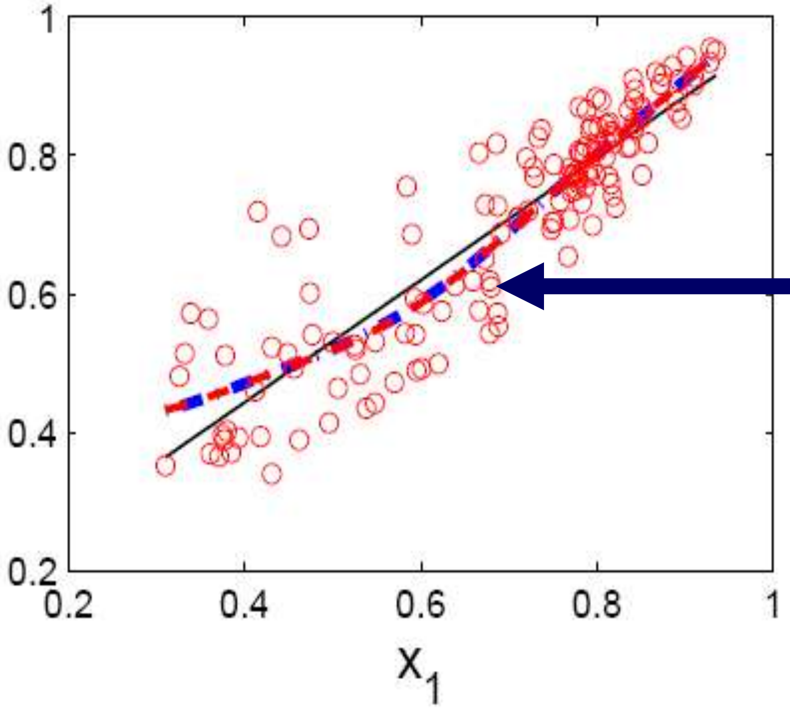
Pearson's correlation ratio

Smoothed curve

$$S_i \equiv \eta_i^2 := \frac{V_{x_i}\left(E_{\mathbf{x}_{\sim i}}\left(y \mid x_i\right)\right)}{V\left(y\right)}$$

First order sensitivity index

Unconditional variance



Smoothed curve

$$E_{\mathbf{x}_{\sim i}}\left(y \mid x_i\right)$$

First order sensitivity index:

$$\frac{V_{x_i}\left(E_{\mathbf{x}_{\sim i}}\left(y \mid x_i\right)\right)}{V\left(y\right)}$$

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right)$$

First order effect, or top marginal variance=

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

Why?

We need first to prove that

$$V(Y)=E(Y^2)-E^2(Y)$$

Because:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right) + E_{X_i}\left(V_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right) = V(Y)$$

Easy to prove using $V(Y)=E(Y^2)-E^2(Y)$

Because:

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right) + E_{X_i}\left(V_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right) = V(Y)$$

This is what variance would be left (on average) if Xi could be fixed…

··· then this ···

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right) +$$

$$+ E_{X_i}\left(V_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right) = V(Y)$$

··· must be the expected reduction in variance that would be achieved if factor Xi could be fixed

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

$$\sum_i V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right) \approx V(Y)$$

… which is also how additive models are defined

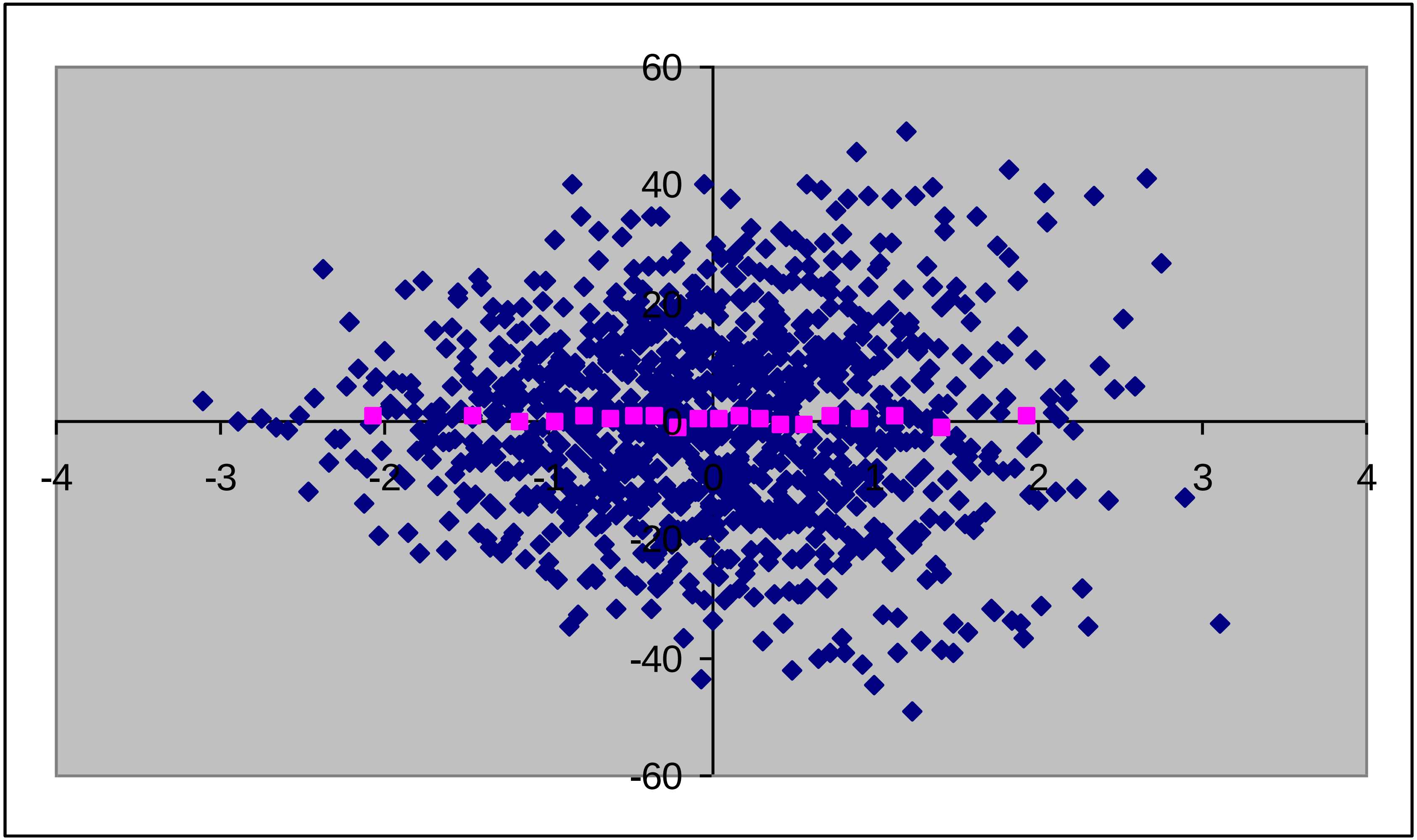
If an additive model is one where the variance V of the output is a linear combination of the partial variances of the inputs then:

- can I guess a formula for an additive model $f(x_1, x_2, x_3, \cdots)$?

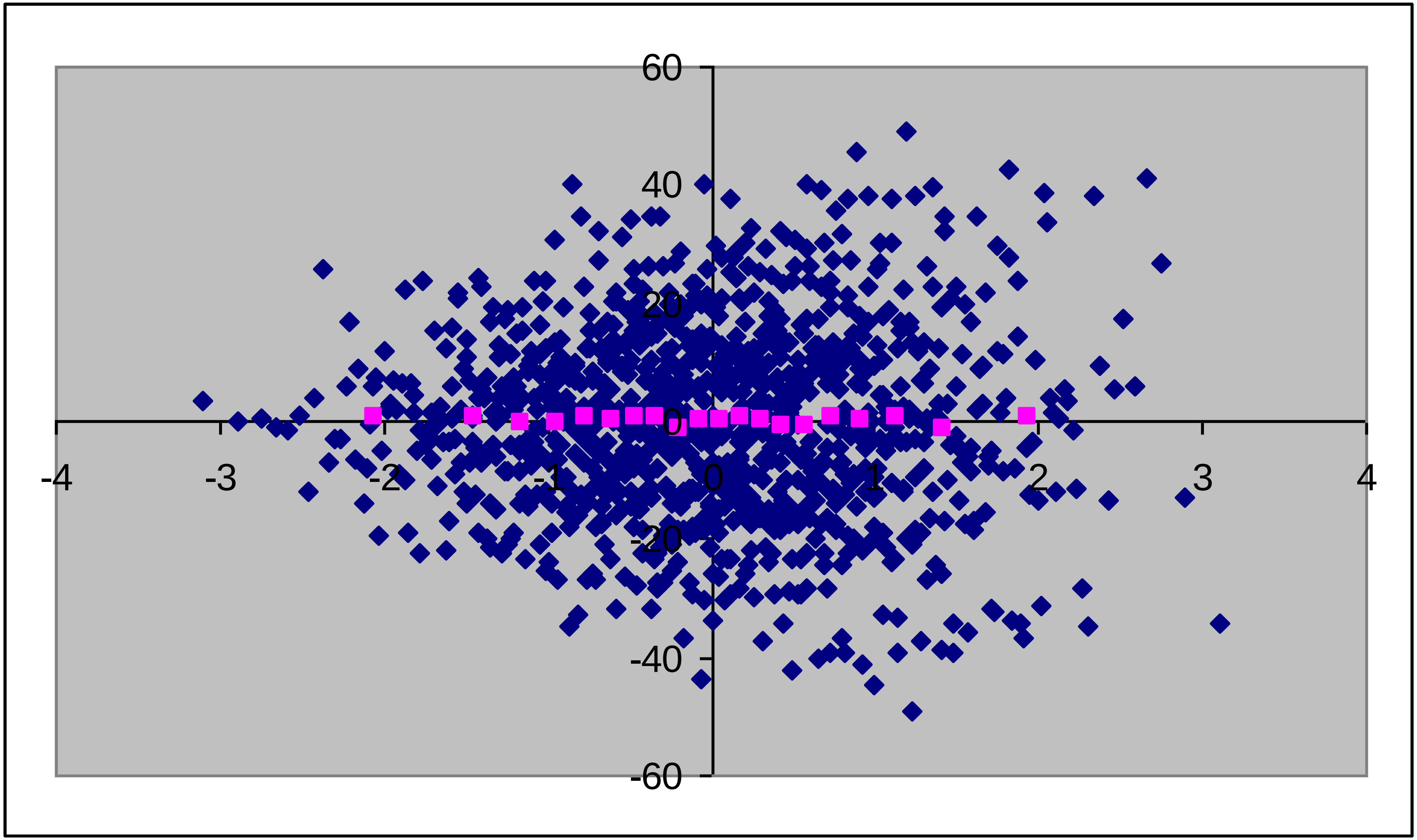
- and for a non additive one?

Non additive models

Is $S_i = 0$?



Is this factor non-important?



There are terms which capture two-way, three way, ⋯ interactions among variables.

All these terms are linked by a formula

Variance decomposition (ANOVA)

$$V(Y) =$$

$$\sum_i V_i + \sum_{i,j>i} V_{ij} + \ldots + V_{123\ldots k}$$

Variance decomposition (ANOVA)

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right) = V_i$$

$$V_{X_i X_j}\left(E_{\mathbf{X}_{\sim ij}}\left(Y \middle| X_i X_j\right)\right) =$$

$$= V_i + V_i + V_{ij}$$

…

Variance decomposition (ANOVA)

When the factors are independent the total variance can be decomposed into main effects and interaction effects up to the order k, the dimensionality of the problem.

Variance decomposition (ANOVA)

When the factors are <u>not</u> independent the decomposition loses its unicity (and hence its appeal)

If fact interactions terms are awkward to handle: second order terms are as many as $k(k-1)/2$ ···

Wouldn’t it be handy to have just a single ‘importance’ terms for all effects, inclusive of first order and interactions?

In fact such terms exist and can be computed easily, without knowledge of the individual interaction terms

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

Instead of

$$V = V_1 + V_2 + V_3 +$$

$$+ V_{12} + V_{13} + V_{23} +$$

$$+ V_{123}$$

which divided by V becomes $\cdots$

$$1 = S_1 + S_2 + S_3 +$$

$$+ S_{12} + S_{13} + S_{23} +$$

$$+ S_{123}$$

We can compute an index S_{Ti} so that e.g. for factor x_1:

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

and analogue formulae for S_{T2}, S_{T3} which can be computed without knowing S_1, S_{12}, S_{13}, S_{123} …

S_{T1} is called a total effect sensitivity index

$$E_{\mathbf{X}_{\sim i}}\left(V_{X_i}\left(Y|\mathbf{X}_{\sim i}\right)\right)$$

Total effect, or bottom marginal variance=

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

$$S_{Ti} \equiv \frac{E\left(V\left(Y \middle| \mathbf{X}_{\sim i}\right)\right)}{V_Y}$$

What is the shortcoming of S_{Ti}?

$$\frac{V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \mid X_i\right)\right)}{V(Y)} = S_i$$

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

Scaled to [0,1]; first order and total order sensitivity coefficient

Why these measures?

$$V_{X_i}\left(E_{\mathbf{X}_{\sim i}}\left(Y \middle| X_i\right)\right)$$

Factors prioritization

$$E_{\mathbf{X}_{\sim i}}\left(V_{X_i}\left(Y \middle| \mathbf{X}_{\sim i}\right)\right)$$

Fixing (dropping) non important factors

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.

More about the settings:

•Factor prioritisation → $$S_i \equiv \frac{V\left(E\left(Y \middle| X_i\right)\right)}{V_Y}$$

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

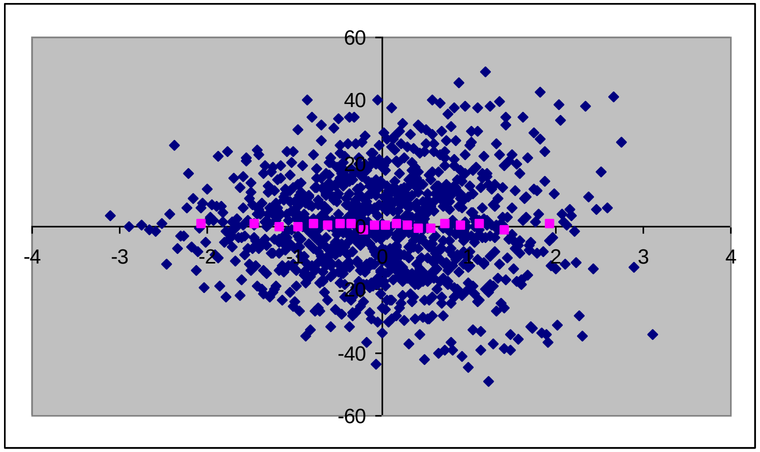
•Factor fixing: Can I fix a factor [or a subset of input factors] at any given value over their range of uncertainty without reducing significantly the output?

$$S_{Ti} \equiv \frac{E\left(V\left(Y \middle| \mathbf{X}_{\sim i}\right)\right)}{V_Y}$$

Factor fixing is useful to achieve model simplification and 'relevance'.

Can we use S_i to fix a factor?

If S_i =0 is X_i a non-influential factor?



We cannot use S_i to fix a factor; $S_i = 0$ is a necessary condition for X_i to be non-influential but not a sufficient one

X_i could be influent at the second order

Can we use S_{Ti} to fix a factor?

If S_{Ti} =0 is X_i a non-influential factor?

$$E_{\mathbf{X}_{\sim i}}\left(V_{X_i}\left(Y|\mathbf{X}_{\sim i}\right)\right)$$

For a mean of non-negative entries to be zero all entries must be zero

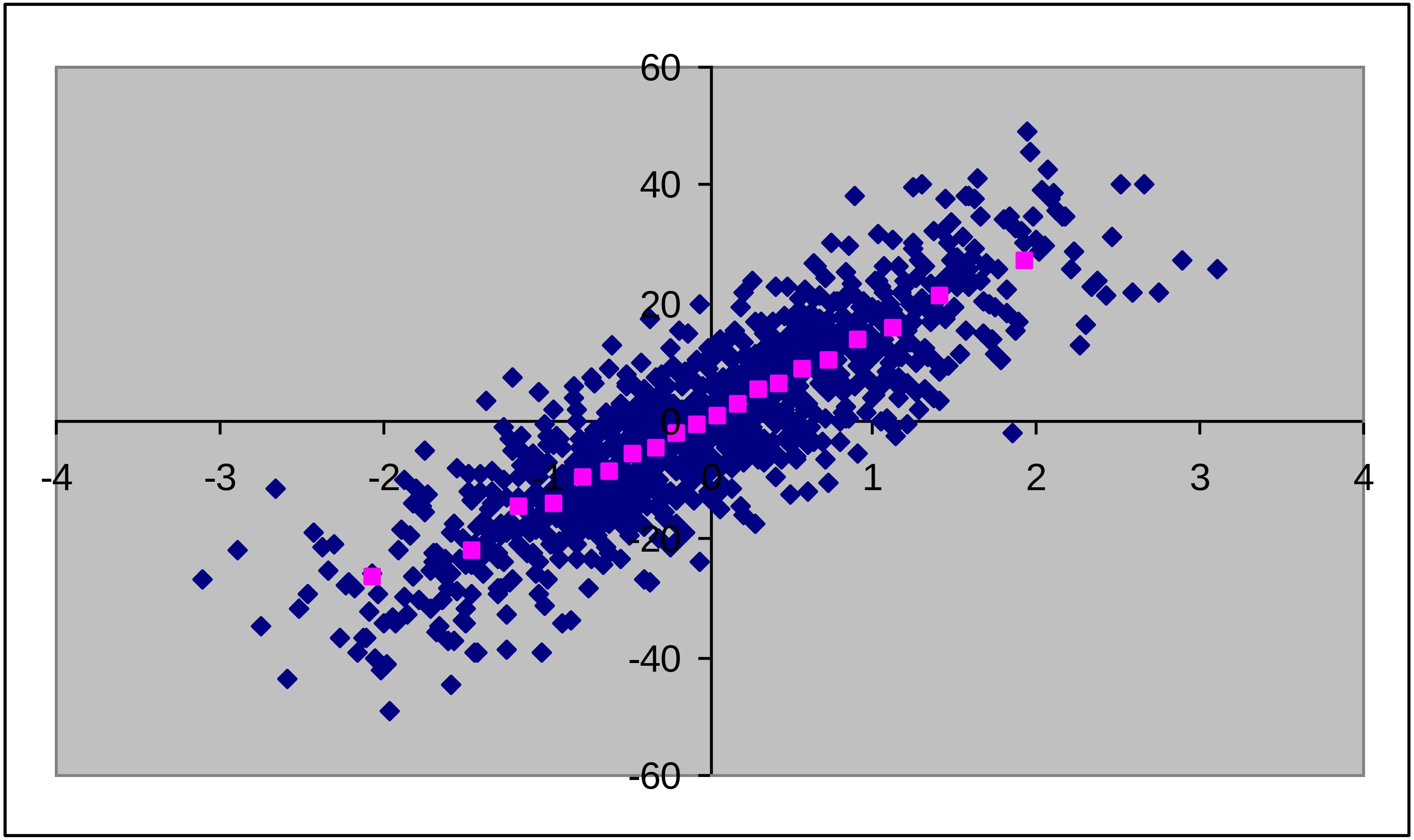
Variance is always a positive number

If $S_{Ti} = 0$ ➔ X_i is non influent as there is no point in the hyperspace of the input where x_i has an effect; $S_{Ti} = 0$ necessary and sufficient condition for non-influence

Summary for variance based measures:

1. Easy-to-code, Monte Carlo – better on quasi-random points. Estimate of the error available.

2. The main effect can be made cheap; its computational cost does not depend upon k.



Easy to smooth and interpolate!

Summary for variance based measures:

3. <u>The total effect</u> is more expensive; its computational cost is $(k+1)N$ where N is one of the order of one thousand (unless e.g. using emulators …).

How about other methods?

Monte Carlo filtering

When to use Monte Carlo Filtering?

When we are interested not in the precise value of the output y but on whether or not this value is ‘permitted’ or forbidden

y_1 NOT OK

y_2 OK

...

y_N NOT OK

If y can be partitioned into ‘ok’ and ‘not ok’ then ⋯

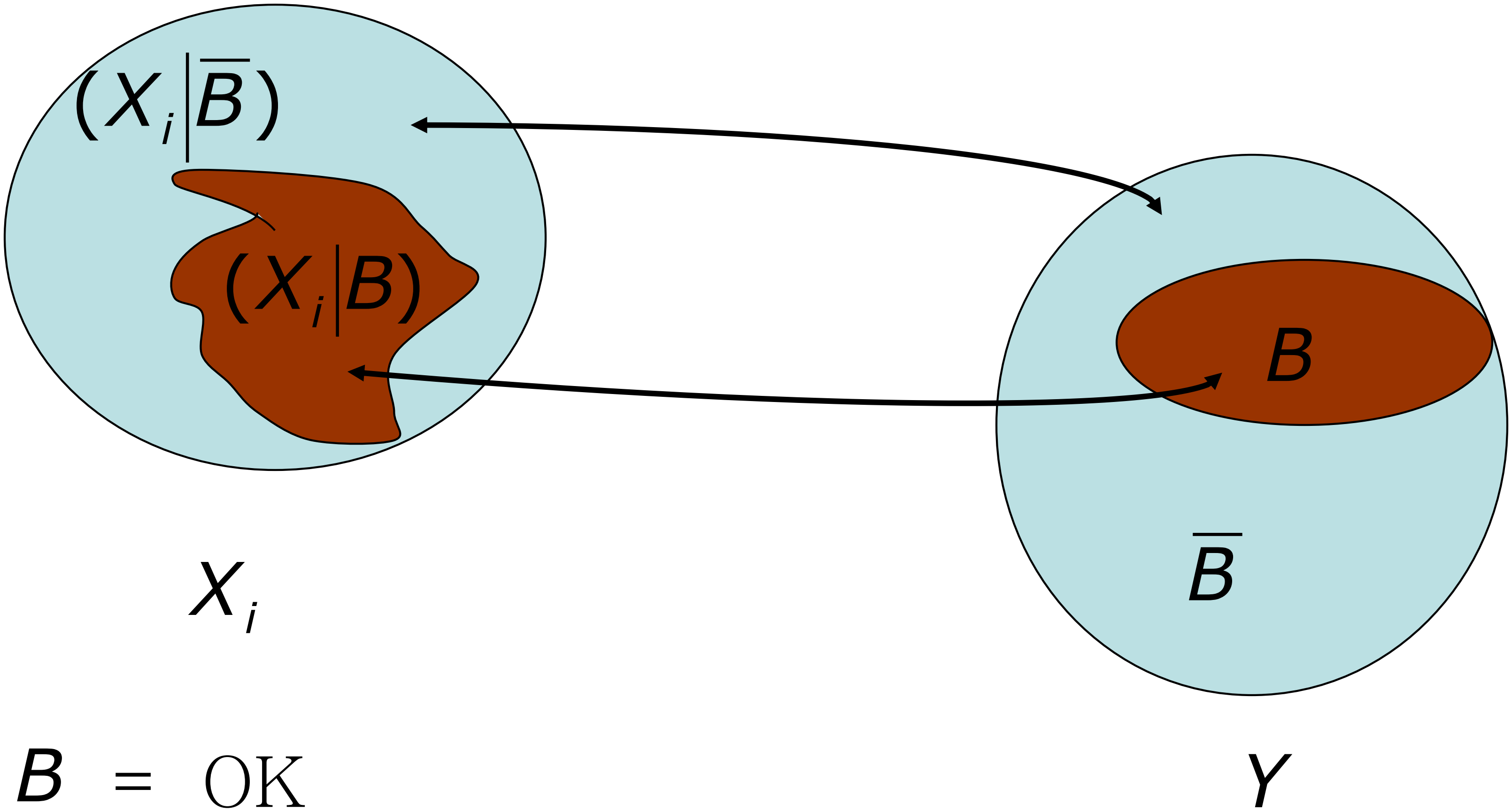
x_{11}	x_{12}	$\cdots$	x_{1k}	NOT OK	y_1	NOT OK
x_{21}	x_{22}	$\cdots$	x_{2k}	OK	y_2	OK
$\cdots$	$\cdots$	$\cdots$	$\cdots$		$\cdots$	
x_{N1}	x_{N2}	$\cdots$	x_{Nk}	NOT OK	y_N	NOT OK

… Then likewise the x_i's can be partitioned; a 'not ok' x_i is one corresponding to a 'not ok' y_i

NOT OK	x_{11}	x_{12}	$\cdots$	x_{1k}
OK	x_{21}	x_{22}	$\cdots$	x_{2k}
	$\cdots$	$\cdots$	$\cdots$	$\cdots$
NOT OK	x_{N1}	x_{N2}	$\cdots$	x_{Nk}

Taking one column at a time I can split the sample of each factor into two subsets

Monte Carlo filtering



B = OK

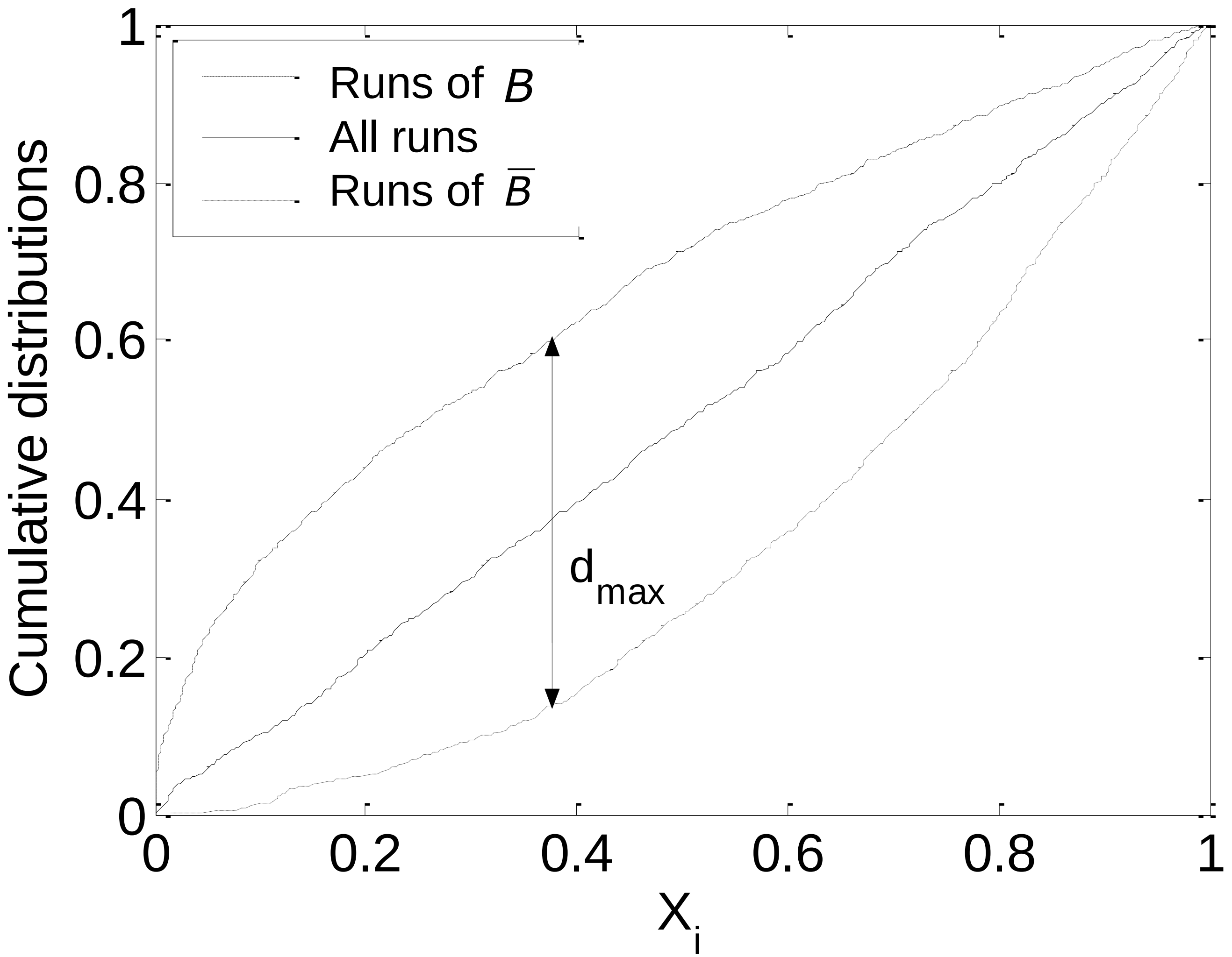
$\overline{B}$ = not OK

Monte Carlo filtering

Step by step:

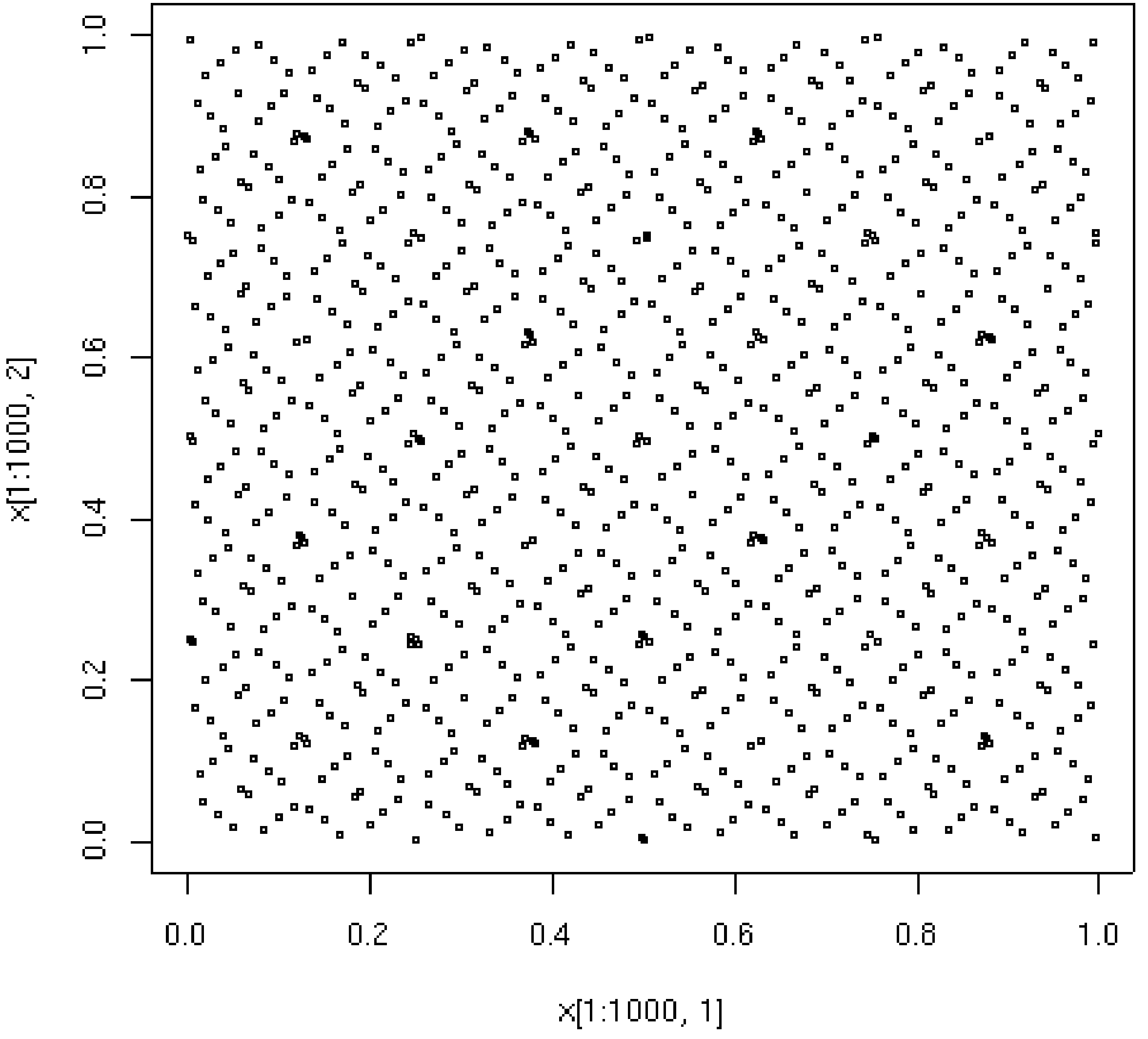
- Classifying simulations as either B or $\bar{B}$. This allows distinguishing two sub-sets for each Xi: $(X_i | B)$ and $(X_i | \bar{B})$
- The Smirnov two-sample test (two-sided version) is performed for each factor independently, analyzing the maximum distance between the cumulative distributions of the B and $\bar{B}$ sets.

Monte Carlo filtering

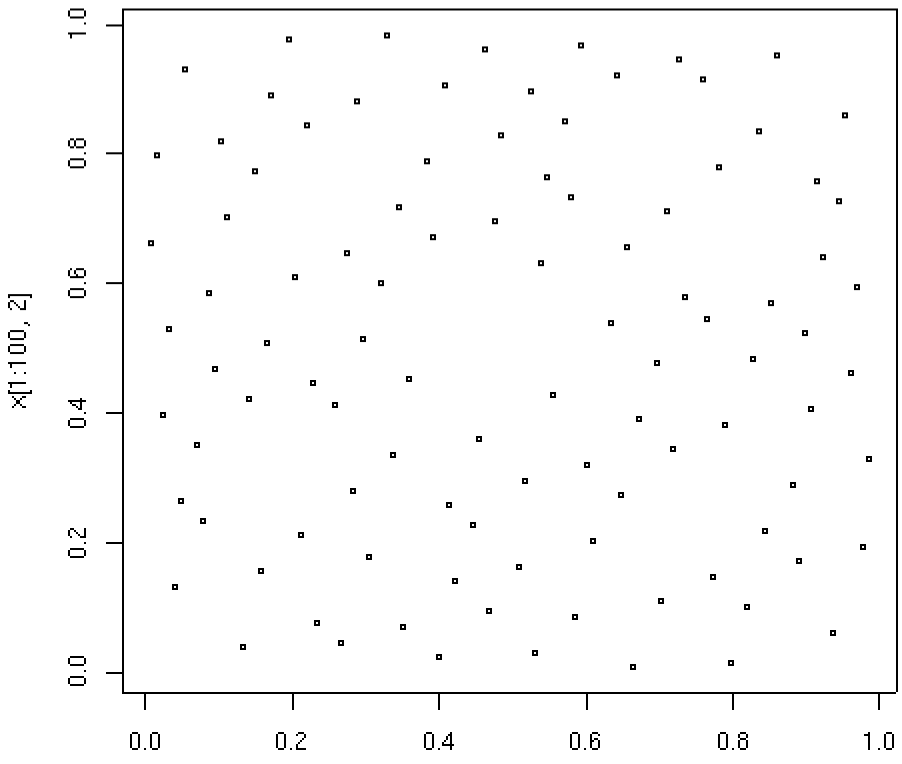


How to generate the random sample?

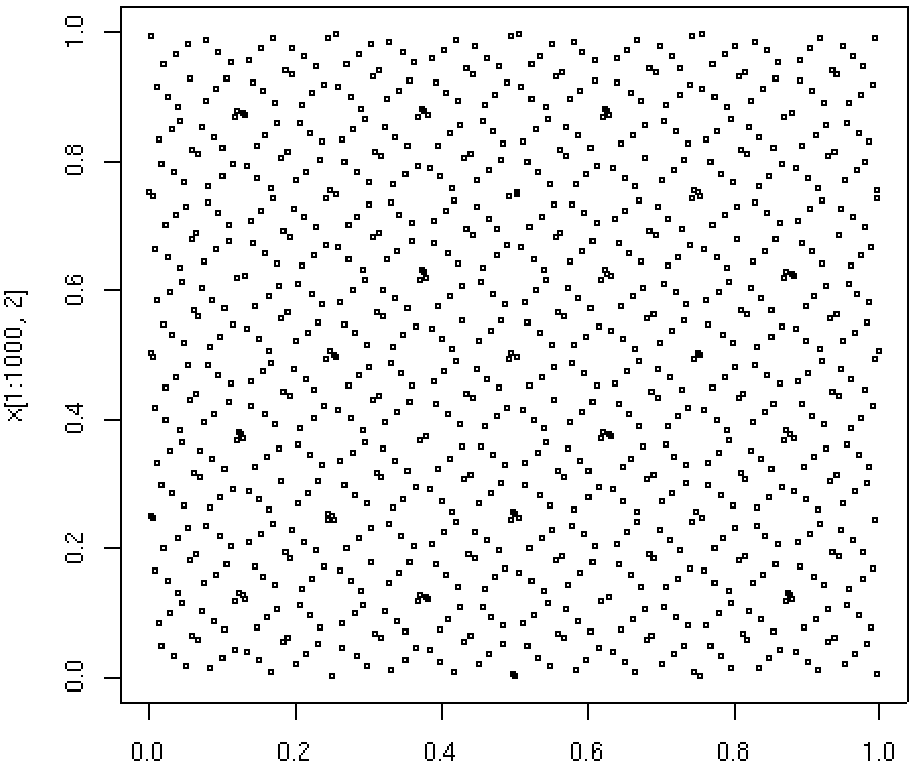
We use quasi random sequences developed by I.M. Sobol'



An LP_τ sequence

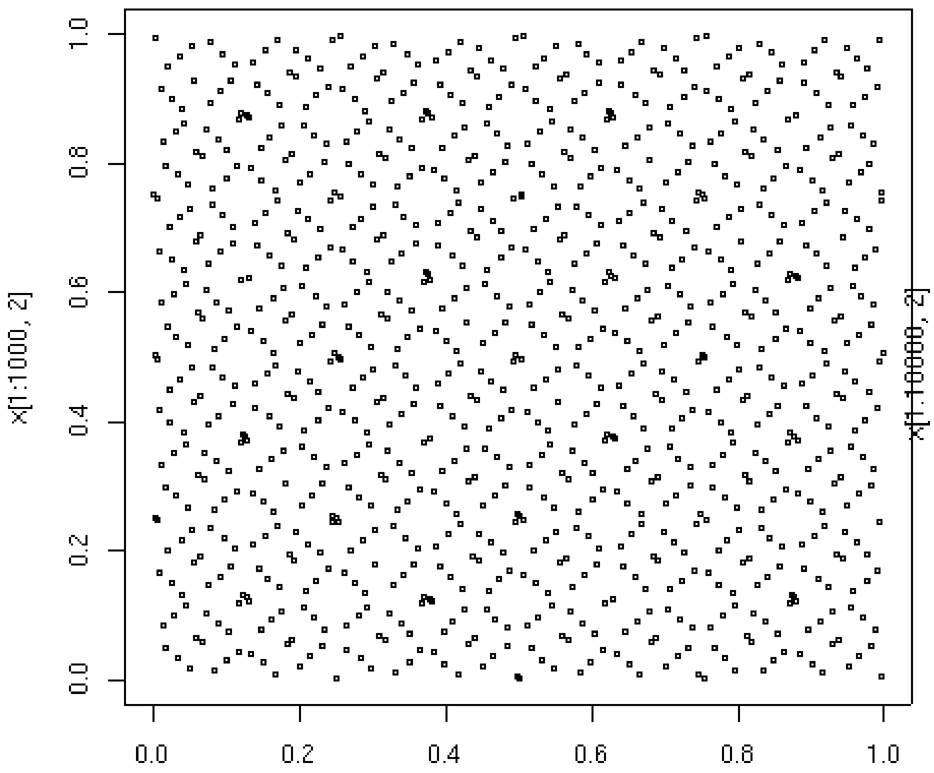


X1,X2 plane, 100 Sobol’ points

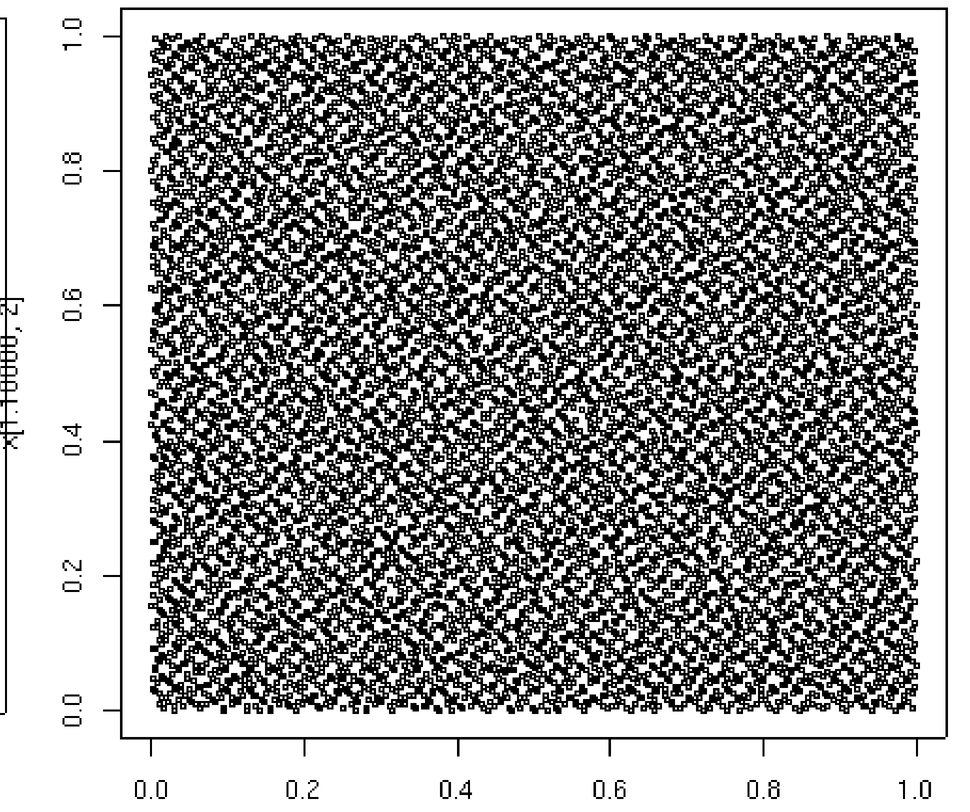


X1,X2 plane, 1000 Sobol’ points

Sobol’ sequences of quasi-random points

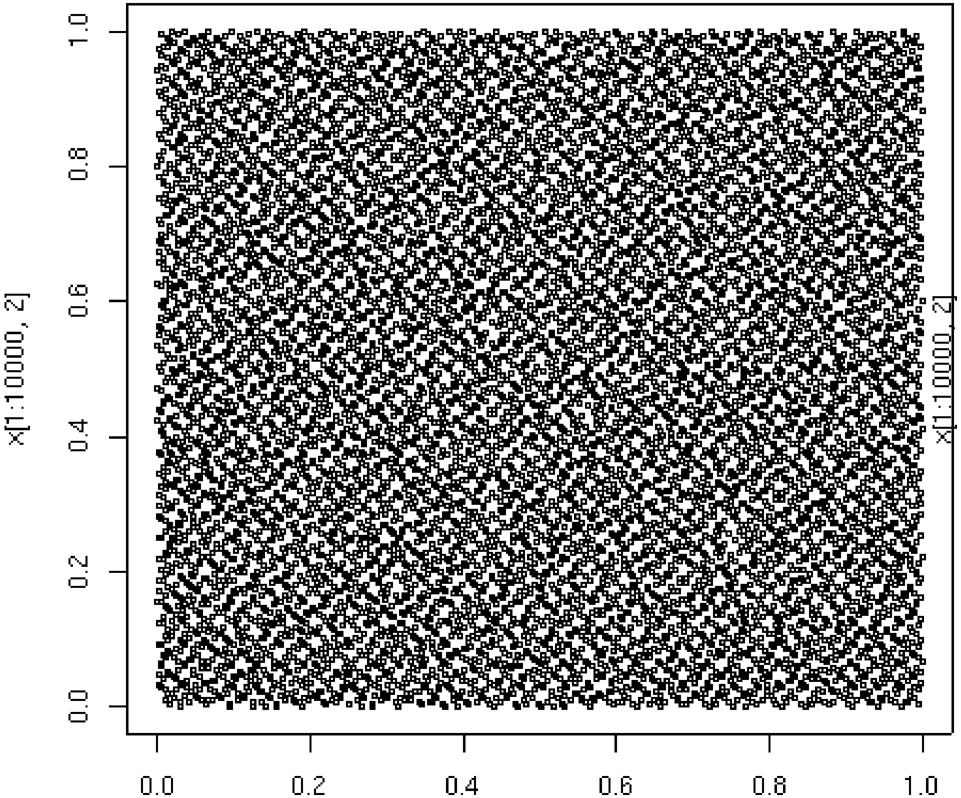


X1,X2 plane, 1000 Sobol’ points

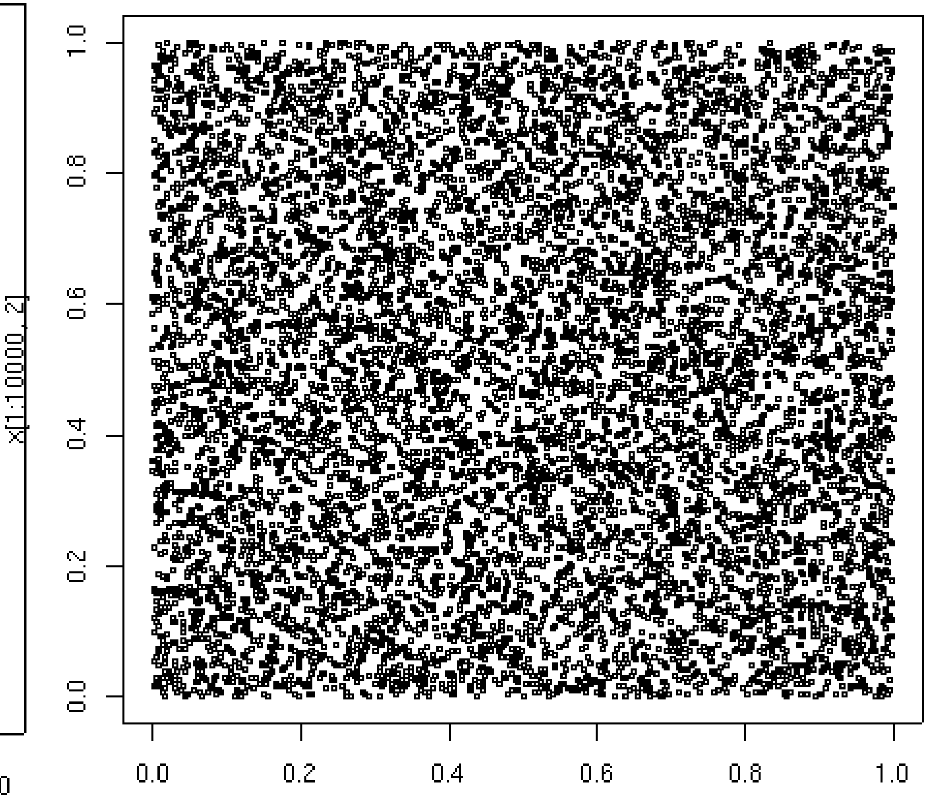


X1,X2 plane, 10000 Sobol’ points

Sobol’ sequences of quasi-random points



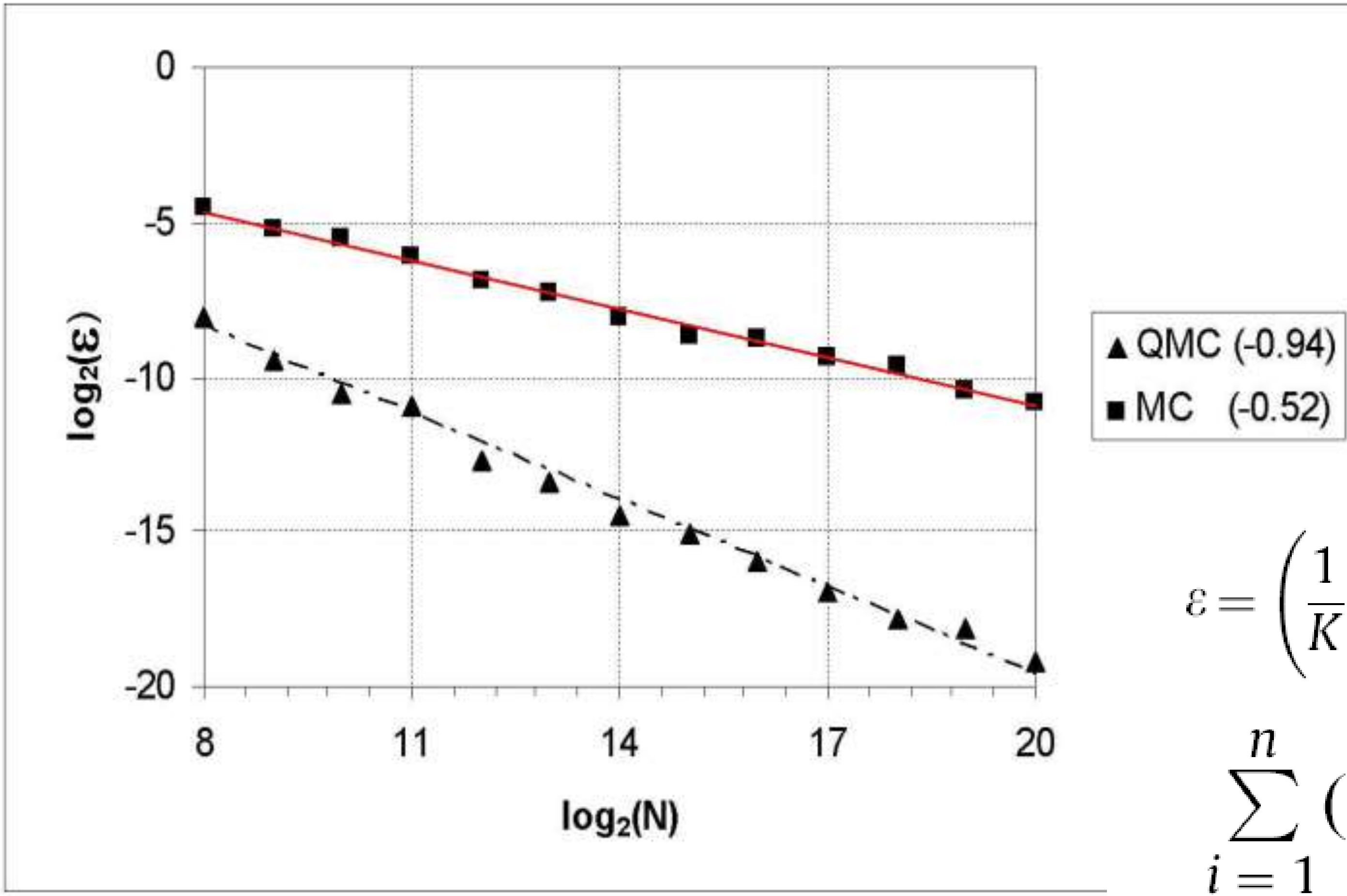
X1,X2 plane, 10000 Sobol' points



X1,X2 plane, 10000 random points

Sobol' sequences of quasi-random points against random points

Why quasi-random



Sergei Kucherenko, Imperial College London

$$\varepsilon = \left(\frac{1}{K} \sum_{k=1}^{K} (I[f] - I_k[f])^2 \right)^{1/2}$$

$$\sum_{i=1}^{n} (-1)^i \prod_{j=1}^{i} x_j$$

Root mean square error over K=50 different trials. The error refers to the numeric-versus-analytic value the integral of the function (for n=360) over its dominion.

Source: Kucherenko S., Feil B., Shah N., Mauntz W. The identification of model effective dimensions using global sensitivity analysis Reliability Engineering and System Safety 96 (2011) 440–449.

Variance based measures are:
-well scaled,
-concise,
-easy to communicate.

Further
- S_i reduces to squared standard regression coefficients for linear model.
- S_{Ti} detect and describe interactions and
- Becomes a screening test at low sample size

See Campolongo F, Saltelli A, Cariboni, J, 2011, From screening to quantitative sensitivity analysis. A unified approach, *Computer Physics Communication*, 182 (4), pp. 978-988.

Secrets of sensitivity analysis

First secret: The most important question is the question.

Corollary 1: Sensitivity analysis is not “run” on a model but on a model once applied to a question.

First secret: The most important question is the question.

Corollary 2: The best setting for a sensitivity analysis is one when one wants to prove that a question cannot be answered given the model

It is better to be in a setting of falsification than in one of confirmation (Oreskes et al., 1994).

[Normally the opposite is the case]

Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences, Naomi Oreskes, Kristin Shrader-Frechette, Kenneth Belitz, Science, New Series, Vol. 263, No. 5147 (Feb. 4, 1994), pp. 641-646.

Second secret: Sensitivity analysis should not be used to hide assumptions
[it often is]

Third secret: If sensitivity analysis shows that a question cannot be answered by the model one should find another question/model which can be treated meaningfully.

[Often the love for the model prevails]

Badly kept secret:

There is always one more bug!

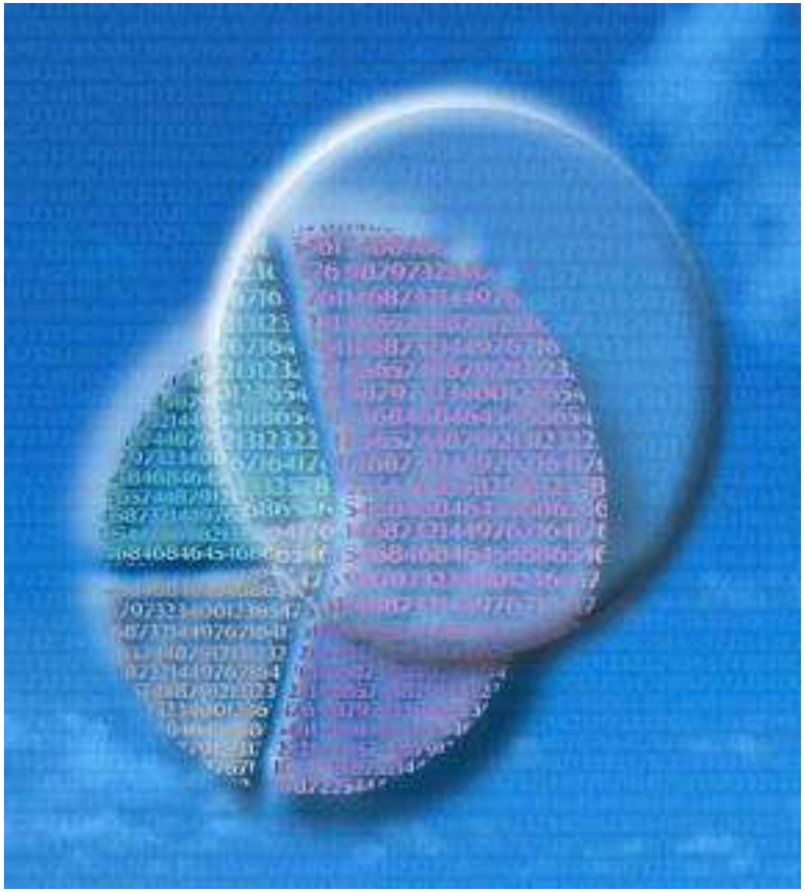
(Lubarsky's Law of Cybernetic Entomology)

And of course please don't …

… run a sensitivity analysis where each factors has a 5% uncertainty

Discussion point

- Why should I not run a sensitivity analysis where each factors has a 5% uncertainty



END

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