Estimating Global Sensitivity Measures: Torturing the Data Until They Confess

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TU Clausthal
St. Étienne, MASCOT-NUM, April 10, 2015

Estimating Global Sensitivity Measures: Torturing the Data Until They ~~Confess~~ Prove Innocent

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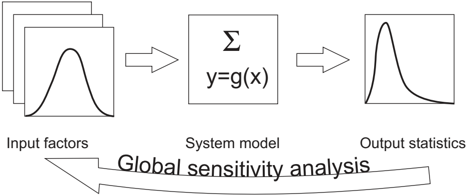
Contents

Global Sensitivity Measures

[Saltelli et al., 2000]
"Sensitivity analysis is the study of how the variation on the output of a model [. . .] can be apportioned [. . .] to different sources of variation, and of how the given model depends upon the information fed into it."
Saltelli in [Faivre et al., 2013]
"Sensitivity analysis is foremost about exploring the space of input assumptions in such a way as to be able to map the inference to the assumptions in a transparent way."



Many Methods Available for Sensitivity Analysis

- Local Methods: Behaviour of the model about a nominal working/reference point
- Screening Methods: Behaviour of the system within given parameter ranges
- Global Methods: Behaviour under given input parameter distributions

Given Data Methodology

X	k-dimensional random vector
Y	random variable (quantity of interest for time series)

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  - But not fast multidimensional/spare grid quadrature designs

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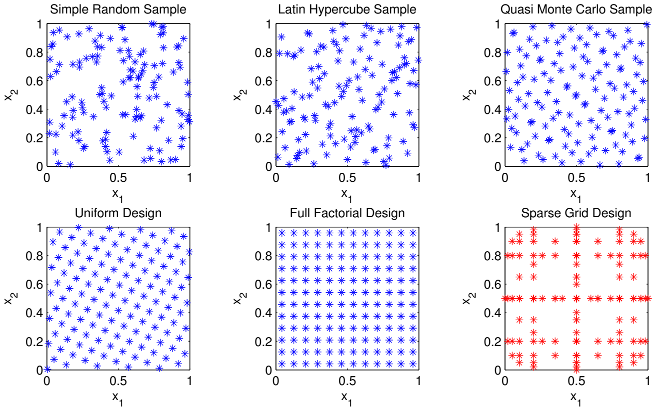
Sample must represent the underlying probabilistic framework.
Observations are independent realizations of (X, Y).

Examples for 2D Uniform [0, 1] Input Samples



Red: Bad setup. But fine for a meta-modeling layer

Why Sample-based?

- Minimal requirements for “design of experiments”
- No model-in-the-loop calculations
- Variable sample size: Fit for computational constraints
- Data re-use: Different sensitivity methods may be applied
- Classical statistical estimators: Bootstrap methods are available
- No functional structure necessary: no strict input/output relation

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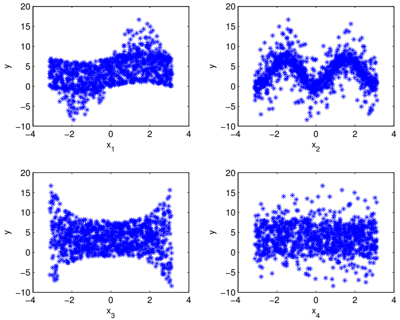
For the rest of the talk

$X = (x_{ij}) \in \mathbb{R}^{n \times k}$ input sample matrix (independent variables),

$Y = (y_i) \in \mathbb{R}^n$ output vector (dependent variable),

Example: The Ishigami test function

$$Y = \sin X_1 + 7\sin^2 X_2 + 0.1 X_3^4 \sin X_1, X_i \sim U(-\pi, \pi) \text{ iid.}$$



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Widely used example

- Only first parameter shows up in linear regression
- First order effects explain just 75% of output variance
- Second order interactions between factors 1 and 3
- Dummy serves as a control

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Visual interpretation of Sensitivity Analysis: Condense the information of a scatterplot into one number!

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Visual interpretation of Sensitivity Analysis: Condense the information of a scatterplot into one number!
In the following: Input factor *j* of interest is fixed – Group effects only touched marginally

Torture Chamber

Painful Least Squares Interrogations

Detecting linear dependence

Correlation between X_j and Y

Sample size			n
x-values			$x_1, \dots, x_i, \dots, x_n$
y-values			$y_1, \dots, y_i, \dots, y_n$
Sums			
x-values		$\Sigma x =$	$x_1 + \dots + x_i \dots + x_n$
y-values		$\Sigma y =$	$y_1 + \dots + y_i \dots + y_n$
x-squares		$\Sigma x^2 =$	$x_1^2 + \dots + x_i^2 \dots + x_n^2$
y-squares		$\Sigma y^2 =$	$y_1^2 + \dots + y_i^2 \dots + y_n^2$
xy-products		$\Sigma xy =$	$x_1 y_1 + \dots + x_i y_i \dots + x_n y_n$
Mean values		$\bar{x} = \frac{1}{n}(\Sigma x)$	$\bar{y} = \frac{1}{n}(\Sigma y)$
Deviances			
	$Sxx =$	$\sum_i (x_i - \bar{x})^2$	$= (\Sigma x^2) - \frac{1}{n}(\Sigma x)^2$
	$Syy =$	$\sum_i (y_i - \bar{y})^2$	$= (\Sigma y^2) - \frac{1}{n}(\Sigma y)^2$
	$Sxy =$	$\sum_i (x_i - \bar{x})(y_i - \bar{y})$	$= (\Sigma xy) - \frac{1}{n}(\Sigma x)(\Sigma y)$
Regression line		$y = \hat{a} + \hat{b}x :$	$\hat{b} = Sxy/Sxx,\ \hat{a} = \bar{y} - \hat{b}\bar{x}$
Correlation coefficient			$\rho = Sxy/\sqrt{SxxSxy}$
Coefficient of determination			$R^2 = (Sxy)^2/(SxxSyy)$

R^2 measures goodness of fit for a linear regression model!

Goodness of Fit – Coefficient of Determination

If $\hat{\varphi}_j(x) = \hat{a}x + \hat{b}$ is the linear regression model for factor j, then

$$R_j^2 = \frac{\mathbb{V}[\hat{\varphi}_j(X_j)]}{\mathbb{V}[Y]} = \frac{\mathbb{E}[(\hat{\varphi}(X_j) - \mathbb{E}[Y])^2]}{\mathbb{E}[(Y - \mathbb{E}[Y])^2]}$$

$\mathbb{V}[\cdot]$	variance
$\mathbb{E}[\cdot]$	expectation

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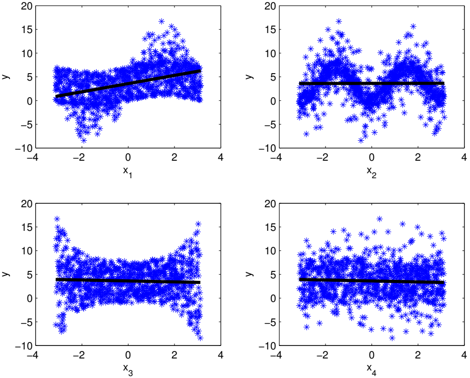
$\mathbb{V}[\cdot]$	variance
$\mathbb{E}[\cdot]$	expectation

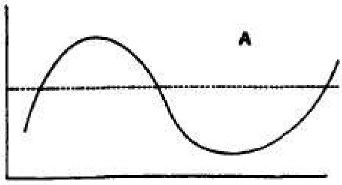
Fraction of the output variance explained by a linear dependence on input factor X_j

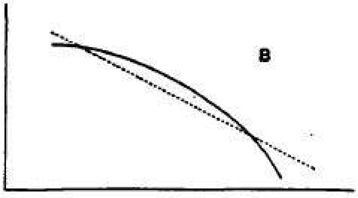
Example: Linear Regression



Parameter	1	2	3	4
R^2	0.1936	0.0000	0.0026	0.0026

But...





[Pearson, 1912]: "Nothing can be learnt of association by assuming linearity in a case with a regression line (plane, etc.) like A, much in a case like B."

Torture Chamber

Stretching and Squeezing with Rank Transformations

Detecting monotonic dependence

Spearman Rank–Correlation

Replace each value with its rank before computing the regression line

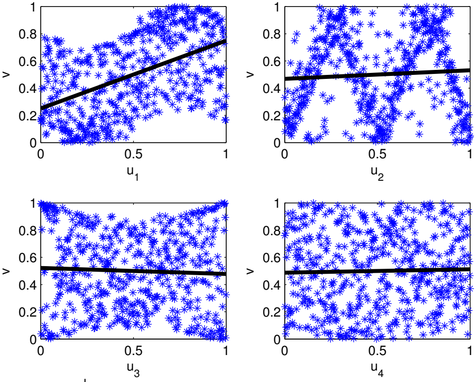
$$Rk(z) = \sum_{i=1}^{n} \mathbf{1}\{z_i \leq z\}$$

Almost the same as the empirical cdf

$$\hat{F}_Z(z) = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}\{z_i \leq z\}$$

Counting the number of realisations smaller or equal to a given value

Example: Rank Regression



Parameter	1	2	3	4
R^{*2}	0.2493	0.0040	0.0019	6.e-04

A Look through the Hidden Backdoor Advanced Instruments

Copula Theory

Study of properties invariant under strictly monotonic transformations [Nelsen, 2006]

A Look through the Hidden Backdoor
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Spearman R^{*2} is just one prominent example

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[Borgonovo et al., 2014]: Many moment-independent sensitivity measures are transformation-invariant (Secret passage to Chamber 4)

Empirical Copula

Already used:

$$(x,y) \mapsto (u,v) \in [0,1]^2, u = \widehat{F}_X(x) = \frac{1}{n}\sum_{j=1}^{n} \mathbf{1}\{x_j \leq x\}, v = \dots$$

Transformation of marginal distributions to uniform

Empirical Copula

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Transformation of marginal distributions to uniform
Same idea in 2D: Empirical bivariate copula

$$\widehat{C}(u, v) = \frac{1}{n}\sum_{j=1}^{n} \mathbf{1}\{u_j \leq u\}\mathbf{1}\{v_j \leq v\}$$

Sensitivity from the Empirical Copula

Under Innocence: $\hat{C}(u, v)$ is a MC integral (relative frequency of hits) of the box area $u \cdot v$

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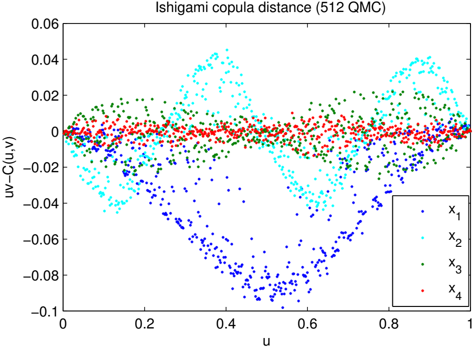
Hence: Compare the independent (product) copula with the empirical copula [Plischke and Borgonovo, 2015]

$$\varphi : u \mapsto uv - \widehat{C}(u, v)$$

Visual tool – Copula distance plots: u vs. $\varphi(u)$

Ishigami Copula Distance: Quasi MC, 512 runs



Spearman ϱ^*	$-12\int_u \varphi(u)du$	$(0.44, 0.00, 0.00, -0.00)$
Schweizer Wolff	$12\int_u \lvert\varphi(u)\rvert\, du$	$(0.44, 0.22, 0.09, 0.03)$
Discrepancy	$4\max_u \lvert\varphi(u)\rvert$	$(0.38, 0.18, 0.10, 0.04)$

Torture Chamber

Slicing into Functional ANOVA Pieces

Detecting functional dependence

Functional ANOVA

$g(\cdot)$ square integrable, $\mathbf{X}$ independent with $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{k} f_i(x_i)$.
Unique representation:

$$g(\mathbf{x}) = \sum_{r=0}^{k} \sum_{\alpha:|\alpha|=r} g_\alpha(\mathbf{x}_\alpha)$$

where $\sum_\alpha$: sum over all subsets of indices of cardinality r.
$g_\alpha(\mathbf{x}_\alpha)$ determined by

$$g_0 = \int_{\mathcal{X}} g(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$g_\alpha(\mathbf{x}_\alpha) = \int_{\mathcal{X}_{\sim\alpha}} \left(g(\mathbf{x}_\alpha, \mathbf{x}_{\sim\alpha}) - \sum_{\beta \subsetneq \alpha} g_\beta(\mathbf{x}_\beta) \right) f_{\sim\alpha}(\mathbf{x}_{\sim\alpha})\,\mathrm{d}\mathbf{x}_{\sim\alpha}$$

where $\mathcal{X}_\beta = \bigotimes_{j\in\beta} \mathcal{X}_j$ and $f_\beta(\mathbf{x}_\beta) = \prod_{j\in\beta} f_j(x_j)$.

Variance Decomposition

For $Y = g(\mathbf{X})$

$$\mathbb{V}[Y] = \sum_{r=1}^{m} \sum_{|\alpha|=r} \mathbb{V}(\alpha) \text{ where } \mathbb{V}(\alpha) = \int_{\mathcal{X}_\alpha} [g_\alpha(\mathbf{x}_\alpha)]^2 f_\alpha(\mathbf{x}_\alpha)\,\mathrm{d}\mathbf{x}_\alpha$$

First order effects	$S_j = \eta_j^2 = \frac{\mathbb{V}(\{j\})}{\mathbb{V}[Y]}$
Total effects	$S_j^T = \sum_{j\in\alpha} \frac{\mathbb{V}(\alpha)}{\mathbb{V}[Y]} = 1 - \sum_{j\notin\alpha} \frac{\mathbb{V}(\alpha)}{\mathbb{V}[Y]}$

Fraction of output variance explained by functional dependence on input factors or groups of input factors.

Sobol' Method

Two independent input samples are mixed to form new samples

$$x_A = \begin{pmatrix} .47 & .09 & .84 & .28 \\ .97 & .59 & .34 & .78 \\ .72 & .34 & .59 & .03 \\ .22 & .84 & .09 & .53 \\ .16 & .16 & .53 & .84 \end{pmatrix} \qquad x_B = \begin{pmatrix} .16 & .84 & .91 & .22 \\ .66 & .34 & .41 & .72 \\ .91 & .09 & .66 & .97 \\ .41 & .59 & .16 & .47 \\ .84 & .66 & .97 & .16 \end{pmatrix}$$

$$x_i = \begin{pmatrix} .47 & .09 & .91 & .28 \\ .97 & .59 & .41 & .78 \\ .72 & .34 & .66 & .03 \\ .22 & .84 & .16 & .53 \\ .16 & .16 & .97 & .84 \end{pmatrix}$$

Associated model output vectors: y_A, y_B and y_i

Sobol' Method II

Correlation coefficient between y_B and y_i:
Sobol' main effect $S_i = \eta_i^2$

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Computational Costs
Each sample block n simulations, given a model with k factors:
$(k+2)n$

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Computational Costs

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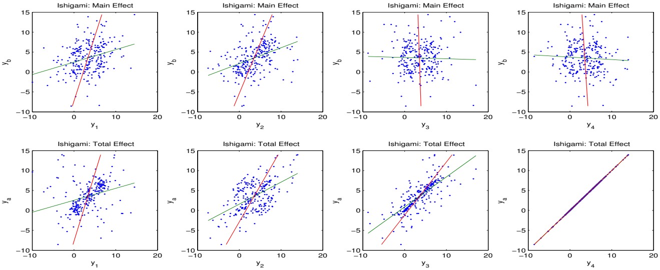
Model in the loop
Sophisticated sample design

Sobol' Method: Correlations for Ishigami



Factor	1	2	3	4
main effect	0.3223	0.4429	-0.0060	-0.0003
total effect	0.5644	0.4427	0.2399	0

Regression Lines: Acute angle $\Longrightarrow$ important main effect or unimportant total effect

First Order/Main Effects from Given Data

Given a nonlinear regression curve for factor j:
$\varphi_j(x) = \hat{\mathbb{E}}[Y|X_j = x]$
Estimation of first order effect $\eta_j^2 = \frac{\mathbb{V}[\mathbb{E}[Y|X_j]]}{\mathbb{V}[Y]}$

$$\hat{\eta}_j^2 = \frac{\sum_{i=1}^n (\varphi_i(x_{ij}) - \bar{y})^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Goodness-of-fit or coefficient of determination, nonlinear R^2
Cost reduction for main effects: From $(k+1)n$ to n
For dependent input samples: no functional ANOVA needed

How to choose φ?

- Affine linear regression models
- Piecewise constant step functions (Pearson, 1905)
- (Piecewise) polynomials, Splines
- Orthogonal polynomial bases (Rabitz & Alış, 1999)
- Harmonic functions (Plischke, 2010)
- Wavelet decompositions
- Moving averages (Doksum & Samarov, 1995)
- LOESS/LASSO/ACOSSO Data Smoothing
- PCA of the output autocovariance, Karhunen-Loéve
- . . .

Cosine Transformation for Sensitivity Indicators [Plischke, 2012b]

For a given sample $(x, y) \in \mathbb{R}^n \times \mathbb{R}^n$

- Let ψ denote the order permutation of x, $x_{\psi(i)} \leq x_{\psi(i+1)}$.

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- Compute cosine transformation frequencies,

$$c_i = \sqrt{\frac{2}{n}} \sum_{j=1}^{n} \cos\left(\frac{\pi(2j-1)i}{2n}\right) y_{\psi(j)}.$$

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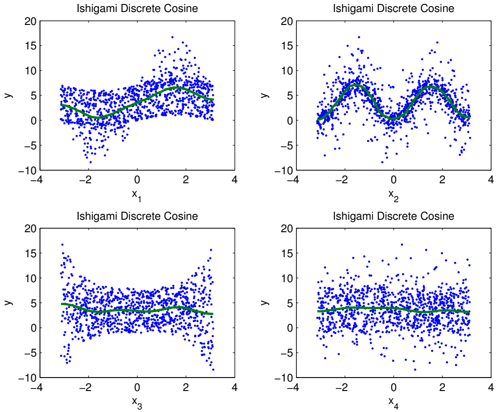
- Gather resonating frequencies,

$$\hat{\eta}^2 = \frac{\sum_{i=1}^{M} c_i^2}{\sum_{i=1}^{n-1} c_i^2}.$$

MATLAB implementation computing first order sensitivity indices

```
 [xr,index]=sort(x);
 yr=y(index); % Reorder output
 allcoeff=dct(yr); % Compute transformation
% Unconditional variance
 V = sum(allcoeff(2:end,:).^2);
% Conditional variance with M resonating harmonics
 Vi= sum(allcoeff(1+(1:M),:).^2);  Si= Vi./V;
```

Cosine sensitivity for the Ishigami example



Parameter	1	2	3	4
η^2	0.3121	0.4333	0.0162	0.0079

Condensing several scatterplots into one figure

Contribution of the input factors to the output mean: Absolute concentration curve, contribution to the sample mean, [Plischke, 2012a]

Cumulative Sum of Normalised Reordered Output (CUSUNORO): Plot the index i against

$$z(i) = \frac{\sum_{j=1}^{i}(y_{\psi(j)} - \bar{y})}{\sqrt{\sum_{j=1}^{n}(y_j - \bar{y})^2}}$$

where $\psi(\cdot)$ is the order permutation for (x_j), $(x_{\psi(j)}) = (x_{(j)})$, $x_{(j)} \leq x_{(j+1)}$.

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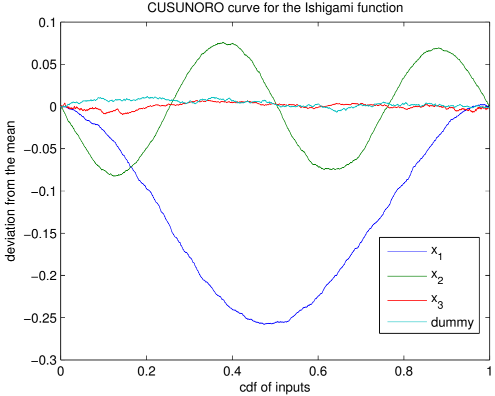
Sample-based version of

$$u \mapsto \frac{1}{\sqrt{\mathbb{V}[Y]}}\mathbb{E}\left[(Y - \mathbb{E}[Y])\mathbf{1}\{X \le F_X^{-1}(u)\}\right]$$

Example: Again Ishigami

Instead of *k* scatterplots: *k* curves in a CUSUNORO plot



Link to First Order Effects

Derivative of CUSUNORO is conditional expectation!
Parameters are sensitive if CUSUNORO deviates from 0-line:
With slight abuse of notation,

$$\hat{\eta}^2 = \int_0^1 (\nabla z(t))^2 \, dt$$

Main effect estimate: Riemann sum of the square of the derivate of the CUSUNORO curve

Sensitivity and Interactions

So far: Methods for estimating first order effects from given data.

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Identification of input factors without influence on the output

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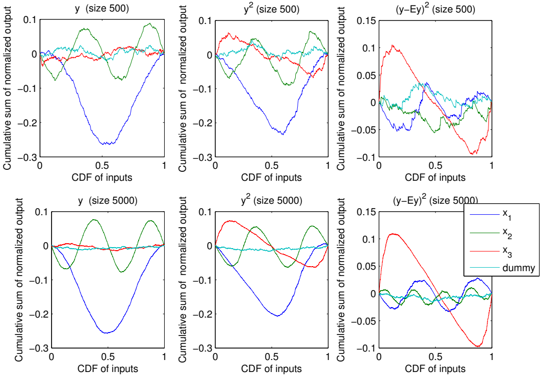
Total effects are important in Factor Fixing Setting -
Identification of input factors without influence on the output
Alternatives

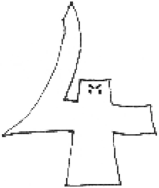
- Higher order effects using generalized regression with feature maps from an orthogonal function basis (HDMR, Polynomial Chaos approach)
- Main effects of higher moments - Replace $y \to (y - \bar{y})^2$
- Compare the probability of Y with the probability of Y conditional to $X_i = x$

CUSUNORO for the second moment



x_3 is sensitive!

Torture Chamber



Iron Maiden of Conditional Piercings

Detecting statistical dependence

General Framework for Sensitivity

A general sensitivity measure

$$\gamma_j(X_j, Y) = \mathbb{E}[\zeta(\mathbb{P}_Y, \mathbb{P}_{Y|X_j})]$$

Suitable distance measure $\zeta(\cdot,\cdot)$: shift/separation/contrast between total and conditional probability measures.

General Framework for Sensitivity

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Suitable distance measure $\zeta(\cdot, \cdot)$: shift/separation/contrast between total and conditional probability measures.

Aswers the question:
What is the (average) value of getting to know that $X_j = x$?

Examples for Shift/Separation/Contrast Functions

$$\zeta_{\mathrm{EI}}(\mu_Y, \mu_{Y|X=x}) = \max\{\mu_{Y|X=x}, 0\} - \max\{\mu_Y, 0\}$$
EVPI, null alternative

$$\zeta_{\mathrm{SI}}(\mu_Y, \mu_{Y|X=x}) = \sigma_Y^{-2}(\mu_Y - \mu_{Y|X=x})^2$$
Main Effect

$$\zeta_{\mathrm{KS}}(F_Y, F_{Y|X=x}) = \sup \left|F_Y - F_{Y|X=x}\right|$$
Kolmogorov-Smirnov

$$\zeta_{\mathrm{Ku}}(F_Y, F_{Y|X=x}) = \sup \left(F_Y - F_{Y|X=x}\right) - \inf \left(F_Y - F_{Y|X=x}\right)$$
Kuiper

$$\zeta_{\mathrm{CvM}}(F_Y, F_{Y|X=x}) = \frac{1}{2}\int \left(F_{Y|X=x}(y) - F_Y(y)\right)^2 dy$$
Cramér, L^2 (cdf)

$$\zeta_{\mathrm{Bo}}(f_Y, f_{Y|X=x}) = \frac{1}{2}\int \left|f_{Y|X=x}(y) - f_Y(y)\right| dy$$
Borgonovo, L^1 (pdf)

$$\zeta_{\mathrm{KL}}(f_Y, f_{Y|X=x}) = \int f_{Y|X=x}(y) \log \frac{f_{Y|X=x}(y)}{f_Y(y)} dy$$
Kullback-Leibler

$$\zeta_{\mathrm{He}}(f_Y, f_{Y|X=x}) = 1 - \int \sqrt{f_Y(y) \cdot f_{Y|X=x}(y)}dy$$
Hellinger

Moment-Independent Sensitivity

The variance of the conditional expectation is is problematic when the output distribution is multi-modal or highly skewed or in case of heteroscedastic data.

Variance works as uncertainty measure only for distributions close to normal.

A moment-independent measure should compare conditional densities/distributions with the unconditional one without recurring to special moments.

Density-Based Sensitivity Measue

Use mean distance between conditional and unconditional densities [Borgonovo, 2007].

$$\delta(X,Y) = \tfrac{1}{2}\,\mathbb{E}[S(X)] = \frac{1}{2}\int_{\mathcal{X}} f_X(x)\int_{\mathcal{Y}} \left| f_Y(y) - f_{Y|X}(y|x) \right| \, dy\, dx$$

δ: L^1-distance of the product of the marginal distributions and the joint distribution

Estimating δ

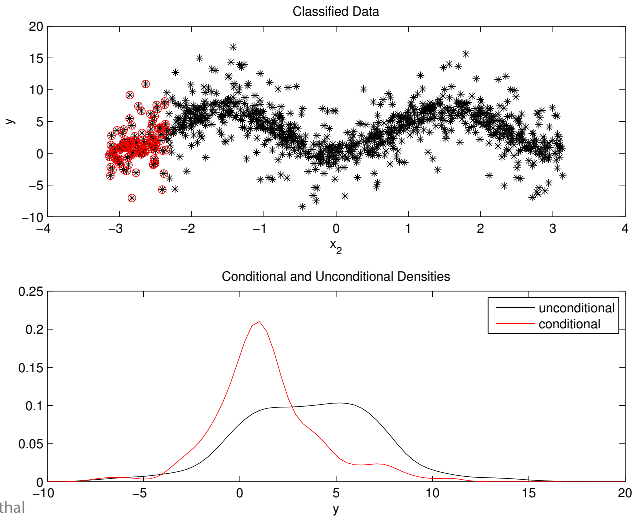
Comparison with variance-based methods:
Instead of conditional expectation $\mathbb{E}[Y|X = x]$: conditional density $f_{Y|X}(y|x)$.

Estimating δ

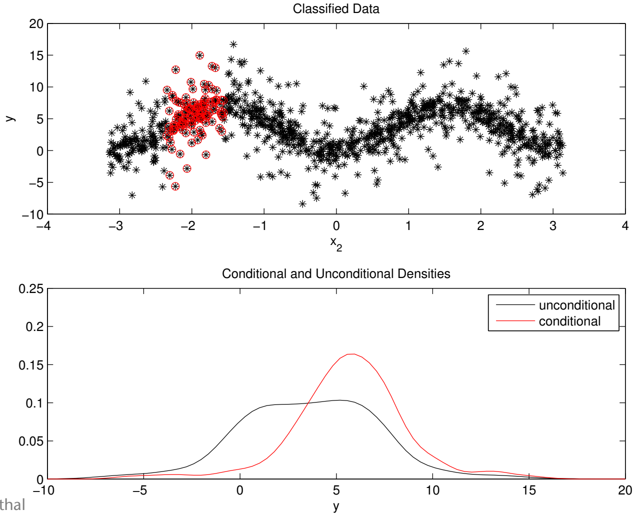
Comparison with variance-based methods:
Instead of conditional expectation $\mathbb{E}[Y|X = x]$: conditional density $f_{Y|X}(y|x)$.

Replace $f_{Y|X=x}(y)$ by $\hat{f}_{Y|X\in\mathcal{C}_r}(y)$ for suitable classes $\mathcal{C}_r$, $r = 1, \ldots, s$, and use kernel density estimation on the classified data $\{y_i|\, x_i \in \mathcal{C}_r\}$ [Plischke et al., 2013]

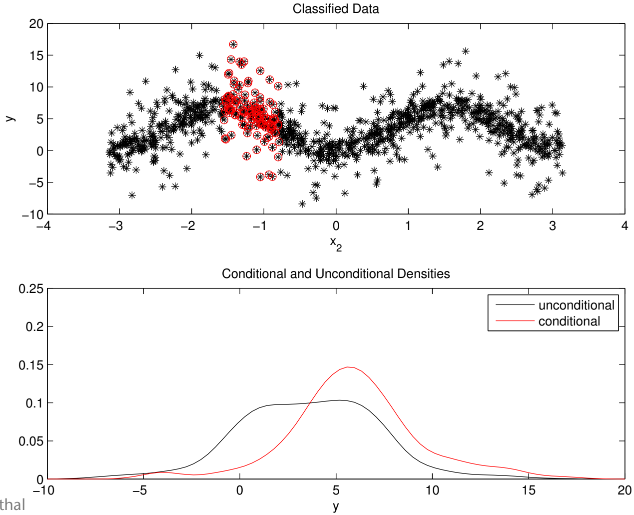
Example: Ishigami Function, Parameter 2



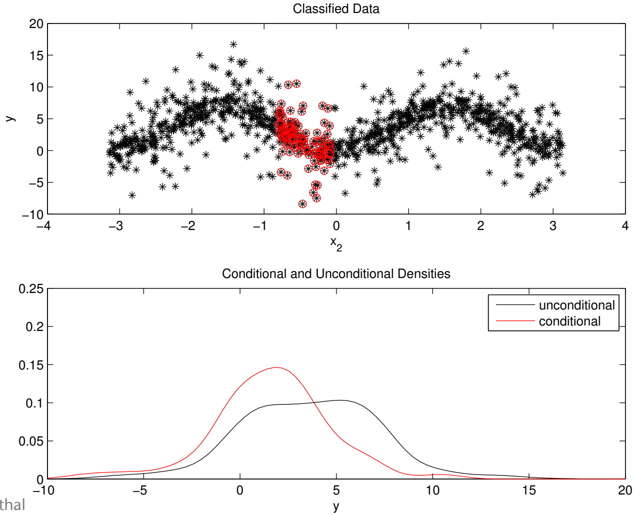
Example: Ishigami Function, Parameter 2



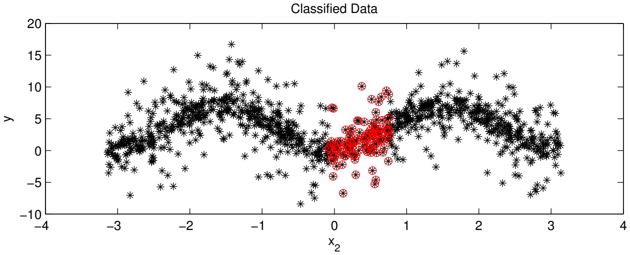
Example: Ishigami Function, Parameter 2

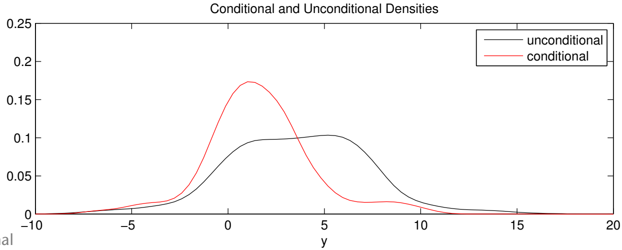


Example: Ishigami Function, Parameter 2

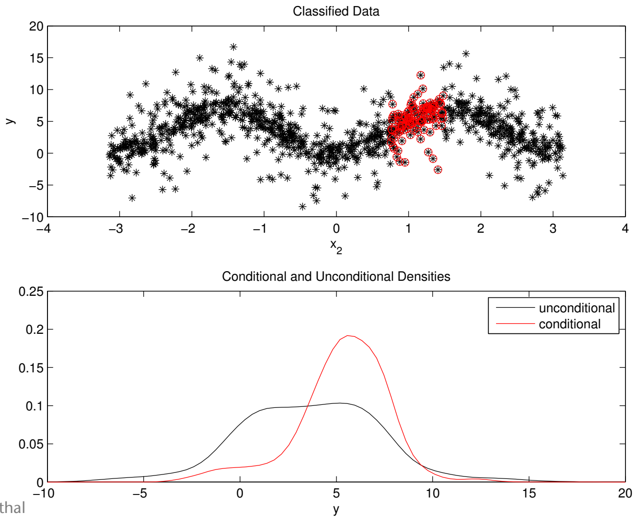


Example: Ishigami Function, Parameter 2

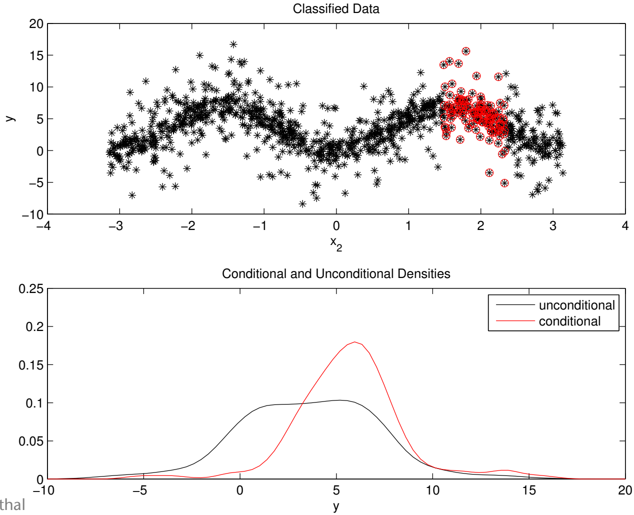




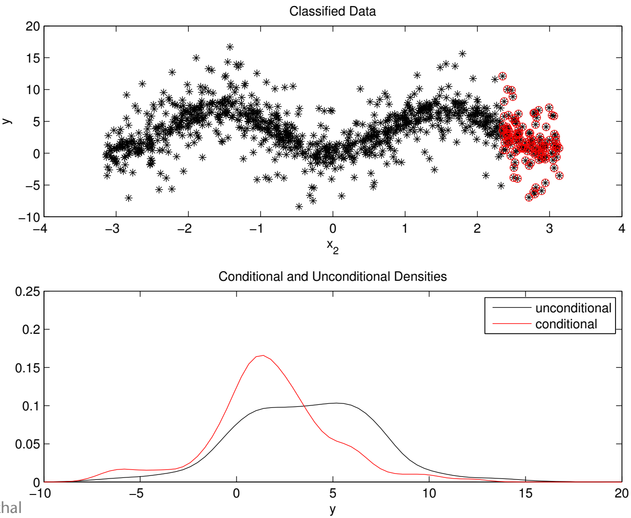
Example: Ishigami Function, Parameter 2



Example: Ishigami Function, Parameter 2



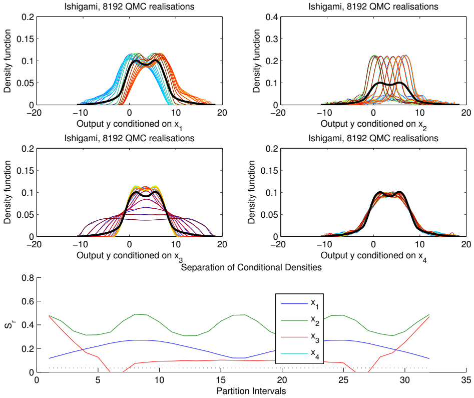
Example: Ishigami Function, Parameter 2



MATLAB Implementation for δ estimation

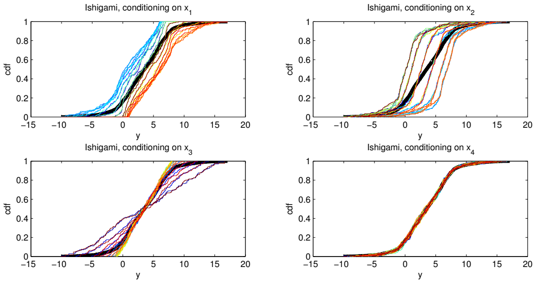
```
Kernel=@(x)3/(4*sqrt(5))*max(1-(x.^2/5),0);[n,k]=size(x);
iqry=median(abs(median(y)-y));
% bandwidth estimate (rule of thumb)
stdy=min(std(y),iqry/(2*0.675)); h=stdy*((4/(3*n))^(1/5));
z=linspace(min(y),max(y),100); % quadrature points
W=Kernel(bsxfun(@minus,z,y)/h)/h; densy=mean(W); %KDE
[xr,indxx]=sort(x);
for i=1:k;   xr(indxx(:,i),i)=1:n; end % ranks
for j=1:M
   indx=((j-1)*n/M<xr) & (xr <= j*n/M);   nm(:,j)=sum(indx);
   for i=1:k
   densc=mean(W(indx(:,i),:)); % conditional density
   Sm(i,j)=trapz(z,max(densy-densc,0)); %only positive part
end
Sm(Sm<Cutoff.*sqrt(1/n+1./nm))=0; d=sum(Sm.*nm,2)'/n;
```

Ishigami Example, 8192 Quasi-MC Samples



Parameter	1	2	3	4
δ	0.2037	0.3918	0.1392	0
η^2	0.3132	0.4365	0.0000	0.0000

Further Moment-Independent Measures

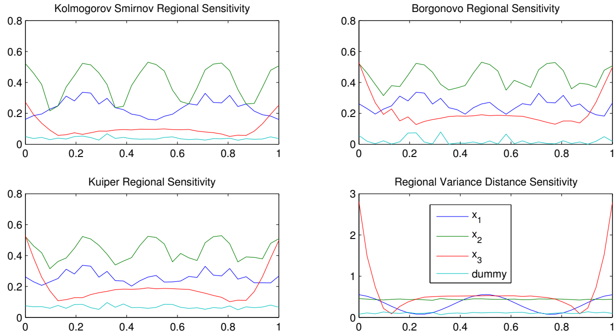


Parameter	1	2	3	4
First Effect η^2	0.3122	0.4321	0.0001	0.0005
Kolmogorov Smirnov β	0.2307	0.3929	0.1018	0.0403
Borgonovo δ	0.2460	0.4213	0.2105	0.0419
Kuiper	0.2525	0.4205	0.1950	0.0694
Wald Wolfowitz	1.6218	2.0463	0.9198	-0.2885

Wald Wolfowitz: Number of conditional subsample runs, normalized

Regional Sensitivity

Plot the separation: $x \mapsto \max_y \left| F_Y - F_{Y|X=x} \right|$ etc.



When to use what?

Sometimes a linear regression provides enough information for a better model understanding.
However, always interpret a sensitivity measure of 0 as inconclusive.

Advantages of linear methods

Small sample of (X, Y) provides info, widely available in software packages

Advantages of variance-based methods

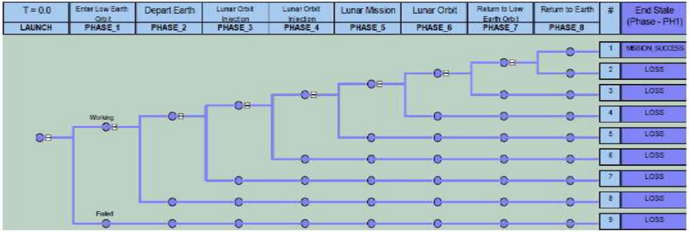
Functional depedence of Y on X detectable

Advantages of moment-independent methods

Indepedence of X and Y $\leftrightarrow$ vanishing indicator

Decision support: NASA lunar mission

Risk assessment of lunar space missions
8-phase process from launch to moon orbit, to return to earth



Decision support: NASA lunar mission

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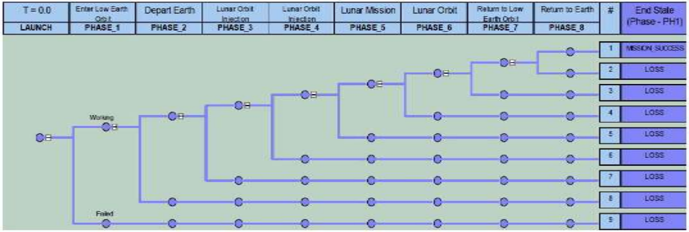
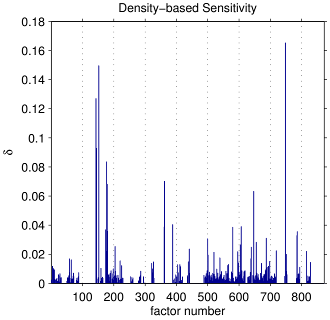
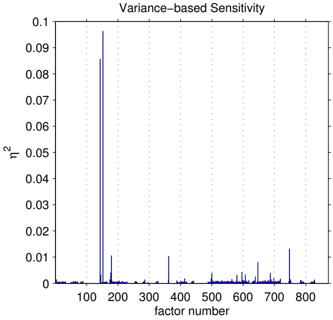


Model is a blackbox processing $k = 872$ uncertain input factors
Crucial: Factors to focus resources in data collection and further modelling efforts

Lunar Mission: Results

QMC sample, 65536×872





Only a few key drivers of uncertainty

Thank You!

Questions, Comments

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Preprints, Scripts, Stuff

http://www.immr.tu-clausthal.de/~epl/

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