Global Sensitivity Analysis with Distance Correlation and Energy Statistics

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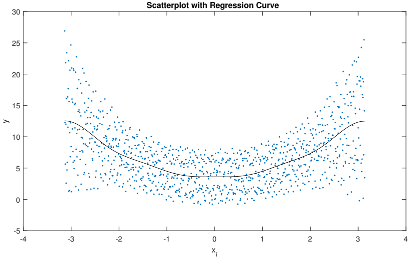
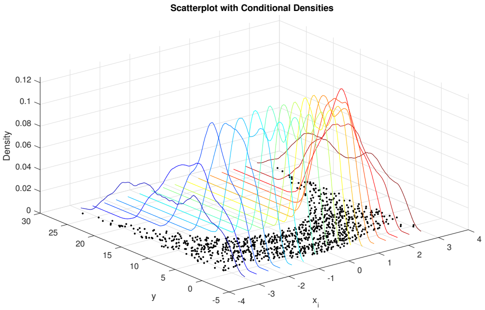


$$S_i = \frac{\mathbb{V}[\mathbb{E}[Y|X_i]]}{\mathbb{V}[Y]},\ \hat{S}_i = \frac{\sum_{j=1}^{n}(\mu_{Y|X_j=x_{ji}} - \mu_Y)^2}{\sum_{j=1}^{n}(y_j - \mu_Y)^2}$$

Conditioning on X_i: Local information from scatterplot

General Framework of Sensitivity Measures

Idea: Replace $(\mu_{Y|X_i=x} - \mu_Y)^2$ by distance measures between Y and $Y|X_i = x$



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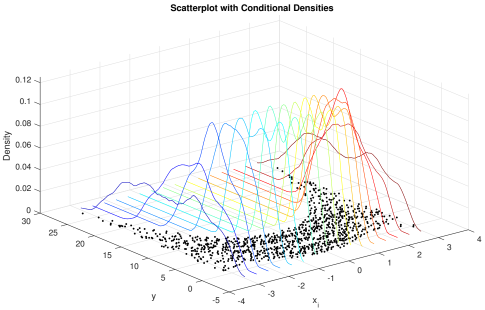

Estimation: Binning the scatterplot into vertical stripes
(interval conditional $Y|X_i \in \mathcal{C}_m^i$ instead of point conditional $Y|X_i = x$)

General Framework II

A general sensitivity measure [Borgonovo et al., 2016]:

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

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

General Framework II

A general sensitivity measure [Borgonovo et al., 2016]:

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

Examples: Shift/Separation/Contrast Functions

$d_{\mathrm{EI}}(\mu_Y, \mu_{Y\|X=x}) = \max\{\mu_{Y\|X=x}, 0\} - \max\{\mu_Y, 0\}$	EVPI, null alternative
$d_{\mathrm{SI}}(\mu_Y, \mu_{Y\|X=x}) = \sigma_Y^{-2}(\mu_Y - \mu_{Y\|X=x})^2$	Main Effect
$d_{\mathrm{KS}}(F_Y, F_{Y\|X=x}) = \sup \left\| F_Y - F_{Y\|X=x} \right\|$	Kolmogorov-Smirnov
$d_{\mathrm{Ku}}(F_Y, F_{Y\|X=x}) = \sup \left(F_Y - F_{Y\|X=x}\right) - \inf \left(F_Y - F_{Y\|X=x}\right)$	Kuiper
$d_{\mathrm{CvM}}(F_Y, F_{Y\|X=x}) = \frac{1}{2} \int \left(F_{Y\|X=x}(y) - F_Y(y)\right)^2 dy$	Cramér, L^2 (cdf)
$d_{\mathrm{Bo}}(f_Y, f_{Y\|X=x}) = \frac{1}{2} \int \left\| f_{Y\|X=x}(y) - f_Y(y) \right\| dy$	Borgonovo, L^1 (pdf)
$d_{\mathrm{KL}}(f_Y, f_{Y\|X=x}) = \int f_{Y\|X=x}(y) \log \frac{f_{Y\|X=x}(y)}{f_Y(y)} dy$	Kullback-Leibler
$d_{\mathrm{He}}(f_Y, f_{Y\|X=x}) = 1 - \int \sqrt{f_Y(y) \cdot f_{Y\|X=x}(y)} dy$	Hellinger

Which one is suitable?

Looking for sensitivity measures which are

- Simple to interpret
- Easy to estimate
- Invariant under monotonic transformations of inputs and outputs
- Detecting strong functional links: $Y = g(X) \implies \mathbb{E}[d(Y, Y|X)] = 1$
- Testing for independence:
  $\mathbb{E}[d(Y, Y|X)] = 0 \iff Y$ and X are independent

No “one–size–fits–all” sensitivity method

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Numerical issues: pdf estimation, extreme values are not numerically stable

Quest for Distance Measures

Candidates should work on whole distribution, not just a point estimate: tests of statistical independence

Here: Closer look at two (and a half) candidates

- Distance Covariance
- Energy Statistics
- (Hilbert Schmidt independence criterion [Gretton et al., 2005])

Studied in SA context: [Da Veiga, 2015, Gamboa et al., 2015, Li et al., 2012]

Distance Covariance and Distance Correlation

At the SIAM UQ 2014 meeting, Grace Wahba (of spline fame) advised the use of Distance Correlation:

"Use Distance Correlation (DCOR) to select a subset of the variables that, taken together are related to the outcome of interest."

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Factor prioritization setting in sensitivity analysis

Distance Covariance

Let X and Y be p and q dimensional random vectors. [Székely et al., 2007] define

$$\mathrm{dCov}(X,Y)^2 = C_{p,q} \iint_{\mathbb{R}^{p+q}} \frac{|\varphi_{XY}(s,t) - \varphi_X(s)\varphi_Y(t)|^2}{\|s\|^{1+p}\,\|t\|^{1+q}} ds dt.$$

$\varphi_{XY}(s,t) = \mathbb{E}[e^{i\langle s,X\rangle + i\langle t,Y\rangle}]$, $\varphi_X(s) = \mathbb{E}[e^{i\langle s,X\rangle}]$, $\varphi_Y(t) = \mathbb{E}[e^{i\langle t,Y\rangle}]$ characteristic functions

$$\mathrm{dCorr}(X,Y) = \frac{\mathrm{dCov}(X,Y)}{\sqrt{\mathrm{dVar}(X)\,\mathrm{dVar}(Y)}}$$

Distance correlation with $\mathrm{dVar}(X) = \mathrm{dCov}(X,X)$

Distance Covariance II

In the scalar case with random variables X and Y:

$$\mathrm{dCov}(X,Y)^2 = \frac{1}{\pi^2}\iint_{\mathbb{R}^2} \frac{|\varphi_{XY}(s,t) - \varphi_X(s)\varphi_Y(t)|^2}{s^2t^2} dsdt.$$

Hence

$$\mathrm{dCov}(X,Y)^2 = \frac{1}{\pi^2}\iint_{\mathbb{R}^2} \left| \frac{\iint e^{i(sx+ty)}\left(f_{XY}(x,y) - f_X(x)f_Y(y)\right)dxdy}{st} \right|^2 dsdt$$

$$= \frac{1}{\pi^2}\iint_{\mathbb{R}^2} \left| \mathbb{E}\left[\frac{e^{isX}}{s}\left(\mathbb{E}\left[\frac{e^{itY}}{t}\middle| X\right] - \mathbb{E}\left[\frac{e^{itY}}{t}\right]\right)\right] \right|^2 dsdt$$

Closely related, but not part of the framework suggested above

Empirical Distance Covariance

For a sample $(x_j, y_j)_{j=1,\dots,n}$ of (X, Y)

$$\widehat{\mathrm{dCov}}(X, Y) = \sqrt{\frac{1}{n(n-3)} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ij}} = \sqrt{\frac{1}{n(n-3)} \operatorname{trace}(AB)}$$

with distance matrices computed via

$$a_{ij} = \left\| x_i - x_j \right\|, \qquad \bar{a}_{i\cdot} = \frac{1}{n-2} \sum_{j=1}^{n} a_{ij}, \qquad \bar{a}_{\cdot j} = \frac{1}{n-2} \sum_{i=1}^{n} a_{ij},$$

$$\bar{a} = \frac{1}{(n-1)(n-2)} \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}, \qquad A_{ij} = a_{ij} - \bar{a}_{i\cdot} - \bar{a}_{\cdot j} + \bar{a}$$

Analogously for (y_j), forming B

Trace product is inner product for vectorized matrices

Hilbert–Schmidt Indepence Criterion

HSIC introduced by [Gretton et al., 2005].
Estimator of HSIC: Absolute values in dCov distances are replaced by kernel evaluations

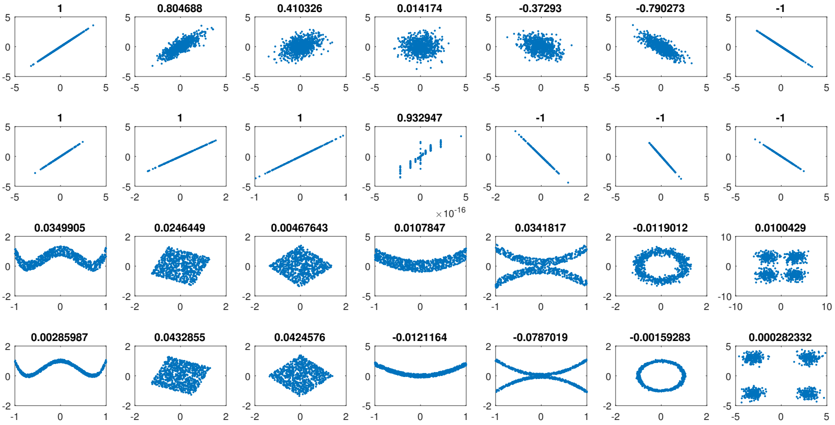
$$a_{ij} = k_X(x_i, x_j), \qquad b_{ij} = k_Y(y_i, y_j)$$

Mostly used with Gaussian kernels

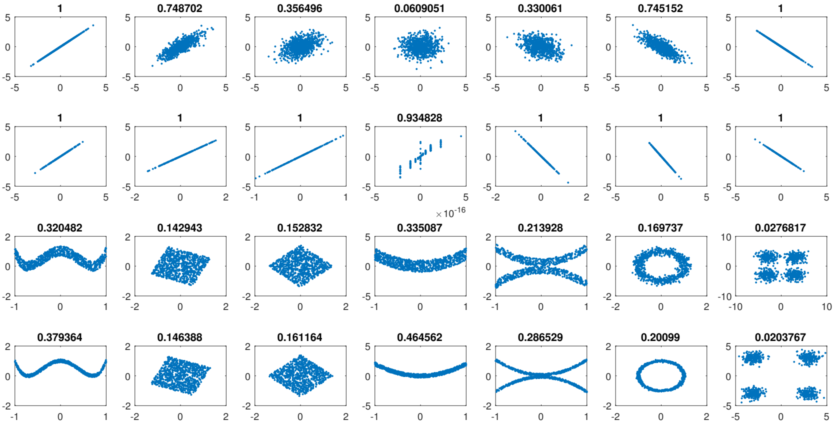
$$k(z_i, z_j) = \exp(-h^{-2}\|z_i - z_j\|^2)$$

Bandwidth h chosen in such way that half of the off-diagonal entries are below e^{-1}
Normalized version: Hilbert–Schmidt Independence Quotient (new)

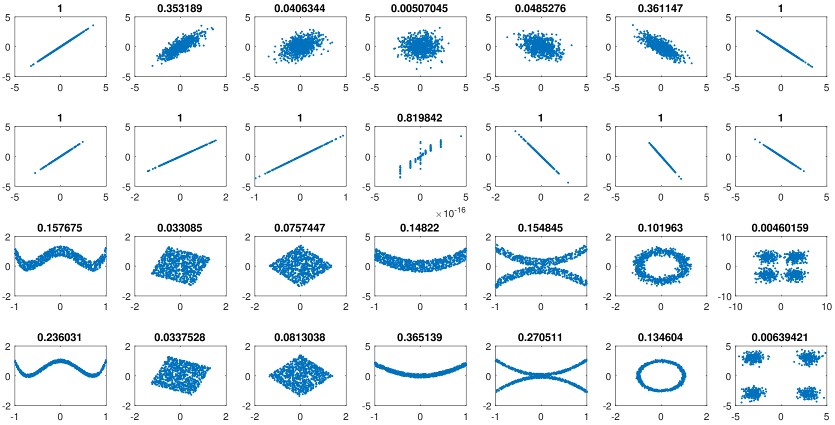
Example: Correlation



Example: Distance Correlation



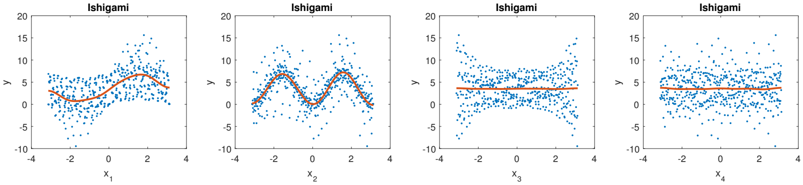
Example: Hilbert Schmidt Independence Quotient



dCov as Sensitivity Measure

Replace correlation with new measure!

Example: Ishigami function with dummy parameter, QMC 512



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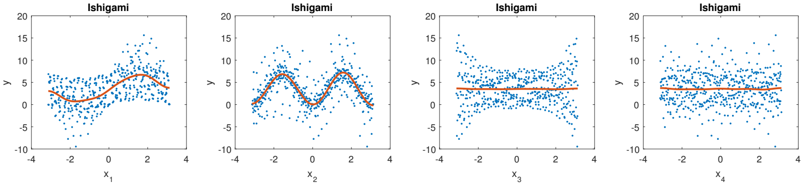

Parameter	Correlation	DCorrelation	First Order Effect
1	0.4304	0.4441	0.3141
2	-0.0043	0.1808	0.4443
3	-0.0018	0.1179	0.0001
4	-0.0013	0.0393	0.0005

dCov as Sensitivity Measure II

- Generalizes linear correlation
- Can detect heteroscedasticity (changing conditional variance)
- Different ranking than from first order effects
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Interaction effects: Consider dCorr($\{X_i, X_j\}, Y$) of Ishigami

$\{i, j\}$	1	2	3	4
1	0.4441	0.3762	0.3612	0.3644
2	0.3762	0.1808	0.1311	0.1023
3	0.3612	0.1311	0.1179	0.0918
4	0.3644	0.1023	0.0918	0.0393

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Interaction sensitivity from dCorr smaller than sum of individual contributions!?
Interactions of factors 1 and 3 not visible! Group sensitivity questionable

Energy Statistics as Sensitivity Measure

For d-dimensional RVecs Y, Z (and iid copies Y', Z') [Székely and Rizzo, 2013] define

$$\mathcal{E}(Y,Z) = 2\,\mathbb{E}\,\|Z - Y\| - \mathbb{E}\,\|Z - Z'\| - \mathbb{E}\,\|Y - Y'\|$$

1D: Gini mean difference $\mathcal{G}(Y) = 2\int F_Y(t)(1 - F_Y(t))dt = 4\,\mathrm{Cov}(Y, F_Y) = \mathbb{E}\,|Y - Y'|$

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Sensitivity framework: $Z = (Y|X=x)$ with separation

$$d(Y, Y|X=x) = \int \Big(F_{Y|X=x}(y) - F_Y(y)\Big)^2 dy = \tfrac{1}{2}\mathcal{E}(Y, Y|X=x)$$
$$= \mathbb{E}\,|(Y|X=x) - Y| - \tfrac{1}{2}(\mathcal{G}(Y) + \mathcal{G}(Y|X=x))$$

Gini (or Cramér–von Mises) sensitivity: $\gamma = \mathbb{E}[d(Y, Y|X)]$

Estimating Energy Statistics

Hoeffding U-statistics (as for dCov): Sample is full of iid copies.
But for large samples: First you run out of patience then you run out of memory.

For 1D: Increasingly sorted output sample $(y_{(j)})$ without ties

$$\widehat{\mathcal{E}}(Y, Y|X_i \in \mathcal{C}_m) = \sum_{j=1}^{n-1} \left(\hat{F}_Y(y_{(j)}) - \hat{F}_{Y|X_i\in\mathcal{C}_m}(y_{(j)})\right)^2 \left(y_{(j+1)} - y_{(j)}\right).$$

By construction $\hat{F}_Y(y_{(j)}) = \frac{j}{n}$, $\hat{F}_{Y|X_i\in\mathcal{C}_m}$ from cumulative sum of the indicator function for $\mathcal{C}_m$

Weighted Energy Statistics

Consider

$$\mathcal{E}^*(Y, Y|X_i = x) = \int \Big(F_Y(y) - F_{Y|X_i=x}(y)\Big)^2 dF_Y(y)$$

$$\widehat{\mathcal{E}}^*(Y, Y|X_i \in \mathcal{C}_m) = \frac{1}{n}\sum_{j=1}^{n-1}\Big(\hat{F}_Y(y_{(j)}) - \hat{F}_{Y|X_i\in\mathcal{C}_m}(y_{(j)})\Big)^2$$

yields transformation-invariant version of Gini measure

$$\gamma^* = 6\iint \Big(F_Y(y) - F_{Y|X_i=x}(y)\Big)^2 dF_Y(y)dF_{X_i}(x)$$

Scale factor: Monotonic dependence yields $\gamma^* = 1$

Weighted Energy Statistics: The Flavour Method of [Gamboa et al., 2015]

- Replace the output Y with quantile indicator functions $1\!\!1\{Y \leq F_Y^{-1}(\theta)\}$
- Compute the variance of the conditional output/first order effects times output variance (scaled by 6) of the indicators
- Average over all quantiles

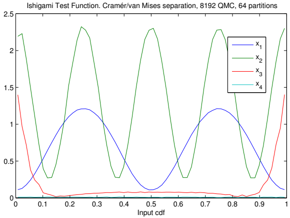
Example: Ishigami 512 QMC, using COSI 10 DCT coefficients vs. partition size 16

Parameter	10%	30%	50%	70%	90%	mean	γ^*	γ
1	.111	.193	.206	.234	.101	.167	0.1789	0.3452
2	.045	.538	.728	.498	.052	.372	0.3399	0.6082
3	.063	.025	.022	.025	.062	.038	0.0347	0.1005
4	.002	.018	.001	.017	.004	.005	0.0147	0.0298

Example: Ishigami

Separation measure for Ishigami (8192 QMC)

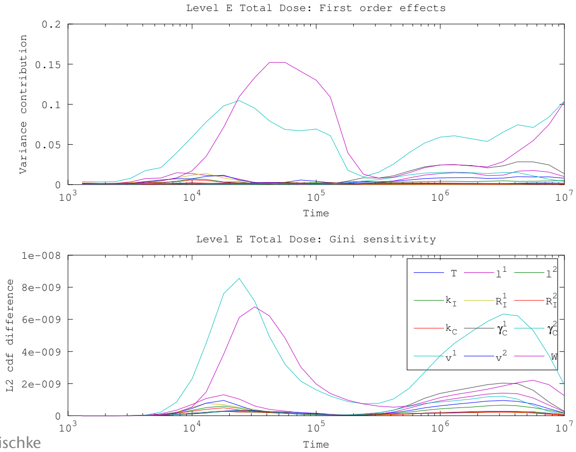
$$\theta \mapsto \widehat{\mathcal{E}}\left((y_j), \left(y_j \middle| \widehat{F}_{X_i}^{-1}(x_{ji}) \in \left[\theta - \frac{1}{M}, \theta\right)\right)\right), \quad \theta = \frac{1}{M}, \ldots, \frac{M}{M}$$



Parameter	1	2	3	4
Gini, 8192 QMC	0.3373	0.6347	0.0822	0.0020
Gini, 512 QMC	0.3807	0.6574	0.1234	0.0526

Example: Geosphere Transport Model Level-E, $k = 12$ inputs

Time-dependent analysis



First order effects: Are all individual contributions accounted for? γ provides additional hints that all indivial factors influencing the conditional distribution (instead of the conditional mean) are being identified.

Conclusions

- Attractive computational schemes
- dCorr: Group interaction may score less than sum of individual contributions?
- Gini / Cramér / von Mises fits into sensitivity framework
- Multidimensional version: Energy statistics
- Transformation-invariant version of Gini / Cramér / von Mises sensitivity
- Prototype software implementations available in MATLAB

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Outlook

- Robust estimation
- Interactions and Group sensitivity

Thank You!

Questions, Comments

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Preprints, Scripts, Stuff

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

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