GLOBAL SENSITIVITY WITH OPTIMAL TRANSPORT

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Motivation

- In several applications model output is multivariate in nature (e.g., vectorial, spatio-temporal dependent)
- We can look at one component at a time
- We also may wish to have an overall indicator of importance

Previous works

- Marrel, Iooss, et al (2011), Models with spatially dependent outputs, Environmetrics.
- Gamboa, Janon, Klein, Lagnoux (2014) Sensitivity Analysis for Multidimensional and Functional Outputs, *Generalized Sobol' Indices*
- Rahman (2016) – The f-sensitivity index (SIAM-JUQ)
- Marrel, Saint-Geours, De Lozzo (2017) in Handbook of Uncertainty Quantification
- Gamboa, Klein, Lagnoux (2018) – Cramer von Mises Distances (SIAM-JUQ)
- Fraiman, R., F. Gamboa, and L. Moreno. 2020. "Sensitivity Indices for Output on a Riemannian Manifold." *International Journal for Uncertainty Quantification* 10 (4): 297–314.

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Previous work (cont.)

- Gamboa, Klein, Lagnoux, Moreno (2021), Sensitivity Analysis in General Metric Spaces: output belongs to a generic metric space
- Fort, Klein, Lagnoux (2021), sensitivity for stochastic outputs when the distance is the Wasserstein distance
- Lamboni (2019), (2020), generalized Sobol' indices and derivative based sensitivity measures
- Alexanderian, Gremaud and Smith (2020) variance-based indices are modified to take into account the temporal variation of the output process variance
- Zham, Constantine, Prieur Marzok, 2020, SIAM J Sc. Comp., with gradient based methods for multivariate vector valued functions
- Da Veiga (2021) (ArXiv) on sensitivity measures based on Kernel-embeddings
- Barr and Rabitz (2022), Siam-JUQ, also on a Kernel-based approach to global sensitivity analysis
- And many others

Optimal transport

- Originated by the work of Gaspard Monge (1781)
- Extended by Kantorovich to a more general formulation (1942)
- Has received increasing attention in mathematics and artificial intelligence
- Distance between images
- Cuturi (2013) breakthrough paper on the solution of the OT problem using the Sinkhorn approximation
- Recent review in SIAM-Review by Chen et al (2021): "Stochastic Control Liaisons: Richard Sinkhorn meets Gaspard Monge on a Schrödinger Bridge"
- Over time two Fields medal Cedric Villani and Alessio Figalli

OT Formulation

— $(\Omega, \mathcal{F}, \mathbb{P})$ reference probability space, let v and v' be two probability measures on this space.

Given $\nu, \nu' \in \mathscr{P}(\mathsf{Y})$ we denote by $\Pi(\nu, \nu')$ the set of plans or couplings $\pi \in \mathscr{P}(\mathsf{Y} \times \mathsf{Y})$ whose marginals are ν and ν' respectively. Posed a lower semicontinuous cost function $\mathsf{k} : \mathsf{Y} \times \mathsf{Y} \to [0, +\infty]$, the Kantorovich formulation of the optimal transport problem

$$K(\nu, \nu') = \inf_{\pi \in \Pi(\nu, \nu')} \mathcal{C}(\pi), \quad \mathcal{C}(\pi) := \int_{\mathsf{Y}^2} \mathsf{k}(y, z)\, \mathrm{d}\pi(y, z), \tag{1}$$

consists of finding a transfer plan $\pi \in \Pi(\nu, \nu')$ that minimizes the integrated cost $\mathcal{C}$.

The Wasserstein Distance

When $\mathsf{k}(y,z) = \mathsf{d}^p(y,z)$ for a suitable continuous metric $\mathsf{d} : \mathsf{Y} \times \mathsf{Y} \to [0,+\infty)$, the Kantorovich problem

$$W_p^p(\nu,\nu') = \inf_{\pi \in \Pi(\nu,\nu')} \int \mathsf{d}^p(y,z)\,\mathrm{d}\pi(y,z) \tag{7}$$

defines the p-th power of the so-called p-Wasserstein distance W_p, which satisfies the axioms of a metric in the subset $\mathscr{P}_p(\mathsf{Y})$ whose measures have finite p-th moment

The Elliptical Distribution Case

In fact, ν and ν' are two normal distributions with mean values μ, μ' and covariance matrices Σ, Σ' respectively, then Givens and Shortt [1984] show that

$$W_2^2(\nu, \nu') = \|\mu - \mu'\|_2^2 + \mathrm{Tr}\left(\Sigma + \Sigma' - 2\left(\Sigma^{1/2}\Sigma'^{1/2}\right)^{1/2}\right), \tag{12}$$

where $\mathrm{Tr}(\cdot)$ denotes the trace of a matrix and $\Sigma^{1/2}$ is the square root of a symmetric and positive matrix. Gelbrich [1990] extends this result for the case in which ν and ν' are two elliptical distributions with the same characteristic generator.

The quantity in Eq. (12) is called the squared Wasserstein-Bures distance

OT-based Global Sensitivity Measures

We define a family of probabilistic sensitivity measures based on optimal transport. We follow the notation in Section 2, and consider an OT-problem with a lower semicontinuous cost function $\mathsf{k} : \mathsf{Y} \times \mathsf{Y} \to [0, +\infty]$ satisfying $\mathsf{k}(y, y') = 0 \;\Leftrightarrow\; y = y'$.

Lemma 2. *Let $\nu, \nu' \in \mathscr{P}(\mathsf{Y})$. The function $K(\cdot, \cdot) : \mathscr{P}(\mathsf{Y}) \times \mathscr{P}(\mathcal{Y}) \to [0, +\infty]$ defined by (1) is a separation measurement and $K(\nu, \nu') = 0 \iff \nu = \nu'$.*

Definition 3. *Let X, Y be random variables with laws μ, ν respectively and let $(\nu_x^{\mathcal{F}})_{x \in \mathsf{X}}$ be the conditional law of Y generated by $(X, \mathcal{F})$. We call*

$$\xi^K(Y, X) := \mathbb{E}[K(\mathbb{P}_Y, \mathbb{P}_{Y|X})] = \int_{\mathsf{X}} K(\nu, \nu_x)\, \mathrm{d}\mu(x) \tag{22}$$

the OT-based global sensitivity measure of X with respect to Y.

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Interpretation

- The most important input is the one for which we expect to spend more work (it is more costly on average) to pass from the distribution of Y to the conditional distribution of Y given X

- The class encompasses several global sensitivity measures. For instance it can be shown that the δ-importance measure (B. 2007) is a special case of an OT-based sensitivity measure if the space of the output is equipped with the discrete metric.

Properties 1: Zero-independence property

Proposition 5. $\xi^K(Y,X) \geq 0$ *and* $\xi^K(Y,X) = 0$ *if and only if* Y *and* X *are statistically independent.*

Properties 2: Functional Dependence

Let:

$$\mathbb{M}_{\mathsf{k}}[Y] := \int_{\mathsf{Y}^2} \mathsf{k}(y, y')\, \mathrm{d}\nu(y)\, \mathrm{d}\nu(y') = \mathbb{E}[\mathsf{k}(Y, Y')]$$

Lemma 6. *For every random variable X, Y*

$$\xi^K(Y, X) \leq \mathbb{M}_{\mathsf{k}}[Y]; \tag{26}$$

in particular ξ^K is finite if $\mathbb{M}_{\mathsf{k}}[Y] < \infty$. In this case, if Y is functionally dependent on X, i.e. $Y = f(X)$ $\mathbb{P}$-a.e. for some Borel map $f : \mathsf{X} \to \mathsf{Y}$, then $\xi^K(Y, X) = \mathbb{M}_{\mathsf{k}}[Y]$ so that the maximum value is attained in (26).

Notable Case

Remark 7. *When* $\mathsf{Y} = \mathbb{R}^m$ *and* $\mathsf{k}(y, y') := |y - y'|^2$ *we have*

$$\mathbb{M}_{\mathsf{k}}[Y] = \int_{\mathsf{Y}^2} |y - y'|^2 \, \mathrm{d}\nu(y) \, \mathrm{d}\nu(y') = 2 \int_{\mathsf{Y}} |y - \bar{\nu}|^2 \, \mathrm{d}\nu(y) = 2\mathrm{Var}[Y], \quad (27)$$

where $\bar{\nu} := \int y \, \mathrm{d}\nu(y) = \mathbb{E}[Y]$. *The previous lemma then yields*

$$\xi^{W_2^2} \leq 2\mathrm{Var}[Y]. \quad (28)$$

In particular ξ^K *is finite if* $\mathbb{E}\left[|Y|^2\right] < \infty$.

A stronger result

Theorem 8. *Assuming* $Y \in L^2(\Omega, \mathbb{P})$, $\xi^{W_2^2}(Y, X) = \mathbb{M}_{\mathsf{k}}[Y] = 2\mathrm{Var}[Y]$ *if and only if there exists a Borel map* $f : \mathsf{X} \to \mathsf{Y}$ *such that* $Y = f(X)$ $\mathbb{P}$*-a.e.*

A New Sensitivity Index

Definition 12. *If* $\mathbb{M}_{\mathsf{k}}[Y] > 0$*, we let*

$$\iota^{\mathsf{k}}(Y,X) = \frac{\xi^{K}(Y,X)}{\mathbb{M}_{\mathsf{k}}[Y]} \tag{32}$$

Based on the results of Section 3.1, we immediately have that for any cost k, $0 \leq \iota^{\mathsf{k}}(Y,X) \leq 1$, with $\iota^{\mathsf{k}}(Y,X) = 0$ indicating statistical independence and $\iota^{\mathsf{k}}(Y,X) = 1$ in the case of functional dependence. In the remainder, we shall focus on the case in which the cost is associated with the squared 2-Wasserstein distance:

$$\iota(Y,X) = \frac{\xi^{W_2^2}(Y,X)}{2\mathbb{V}[Y]}. \tag{33}$$

With this choice, $\iota(Y,X) = 1$ is equivalent to functional dependence.

The Wasserstein-Bures Case

Proposition 13. *Assume that the second moment of Y is finite. If $\mathbb{P}_Y$ is elliptical with generating function h, and $\mathbb{P}_{Y|X}$ is elliptical with the identical generating function h for all values X, then*

$$\iota(Y,X) = \frac{\mathbb{E}[\|\mathbb{E}[Y] - \mathbb{E}[Y|X]\|_2^2] + \mathbb{E}[\mathrm{Tr}\left(\Sigma_Y + \Sigma_{Y|X} - 2\left(\Sigma_Y^{1/2}\Sigma_{Y|X}\Sigma_Y^{1/2}\right)^{1/2}\right)]}{2\mathbb{V}[Y]}, \qquad (34)$$

where the right hand side of (59) is the squared Wasserstein-Bures distance between $\mathbb{P}_Y$ and $\mathbb{P}_{Y|X}$.

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Advective and Diffusive Parts

- The previous index is the sum of two parts:

$$\mathrm{Adv}_X = \frac{\mathbb{E}[\|\mathbb{E}[Y] - \mathbb{E}[Y|X]\|_2^2]}{2\mathbb{V}[Y]},$$

- That accounts for the shift in mean values (centers of mass), and

$$\mathrm{Diff}_X = \frac{\mathbb{E}[\mathrm{Tr}\left(\Sigma_Y + \Sigma_{Y|X} - 2\left(\Sigma_Y^{1/2}\Sigma_{Y|X}\Sigma_Y^{1/2}\right)^{1/2}\right)}{2\mathbb{V}[Y]}.$$

- That accounts for multi-directional dispersion around the means

Link to Gamboa et al Generalized Indices

Proposition 14. *For Adv_X in (36), we have:*

$$Adv_X = \mathbb{E}\left[\|\mathbb{E}[Y] - \mathbb{E}[Y|X_i]\|_2^2\right] = \mathbb{E}\left[\sum_{t=1}^{n_Y}(\mathbb{E}[Y_t] - \mathbb{E}[Y_t|X_i])^2\right] = \sum_{t=1}^{n_Y}\xi_i^{V,t}, \qquad (38)$$

where $\xi_i^{V,t}$ is the univariate variance-based sensitivity measure (19) of X_i with respect to Y_t. Moreover, if we assume that the inputs are independent then we have $Adv_X = \sum_{t=1}^{n_Y}\mathbb{V}[Y^t]S_X^t$, where S_X^t is the Sobol' first order sensitivity measure of X with respect to the t^{th} component of the output, Y^t.

Thus we have a variance contribution, plus other contributions in an OT-based sensitivity measure. If distributions are elliptical, we know the additional term, otherwise we have to solve the OT problem

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Distortion

Theorem 10. *Let* $(\mathsf{Z}, \mathcal{G})$ *be a measurable space and let* $g : \mathsf{X} \to \mathsf{Z}$ *be a* $(\mu, \mathcal{G})$*-measurable map with* $Z := g \circ X$*. We have*

$$\xi^K(Y, X) \geq \xi^K(Y, Z) = \xi^K(Y, (X, \mathcal{F}')), \text{ where } \mathcal{F}'^{-1}(\mathcal{G}) \subset \mathcal{F}. \tag{30}$$

In particular, if the σ*-algebra generated by* g *coincides with* $\mathcal{F}$ *we have* $\xi^K(Y, X) = \xi^K(Y, Z)$.

Monotonicity

Theorem 11. *Let* $(\mathfrak{F}^n)_{n\in\mathbb{N}}$ *be an increasing family of sub-*σ*-algebras in* $\mathfrak{F}$ *with* $\mathfrak{F} = \bigvee_{n=1}^{\infty} \mathfrak{F}^n$*. We have*

$$\lim_{n\to\infty} \xi^K(Y,(X,\mathfrak{F}^n)) = \xi^K(Y,(X,\mathfrak{F})). \tag{31}$$

ESTIMATION

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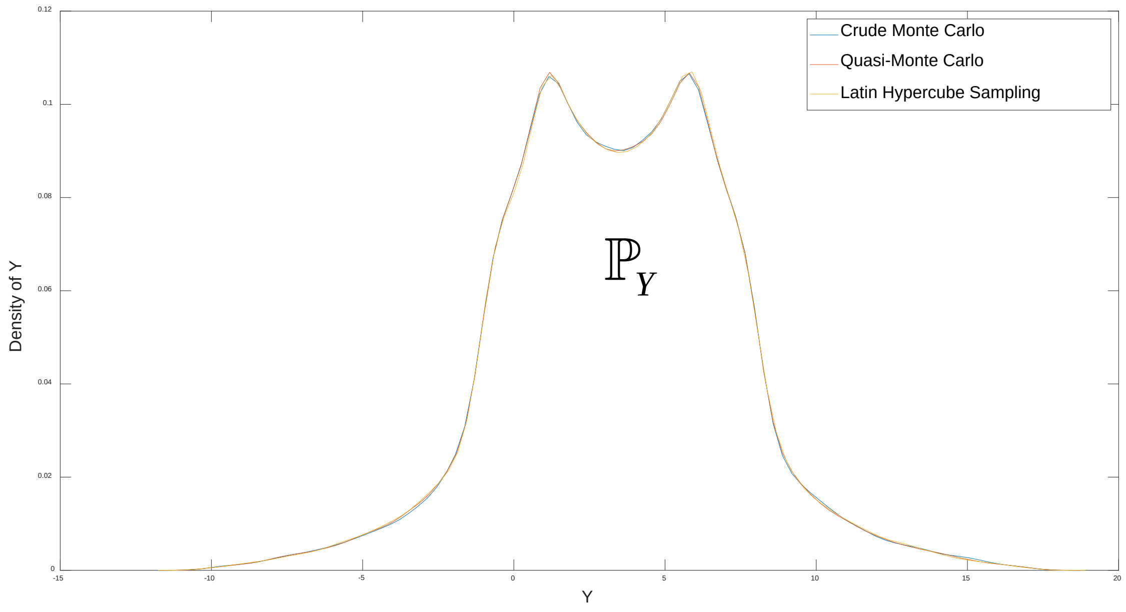
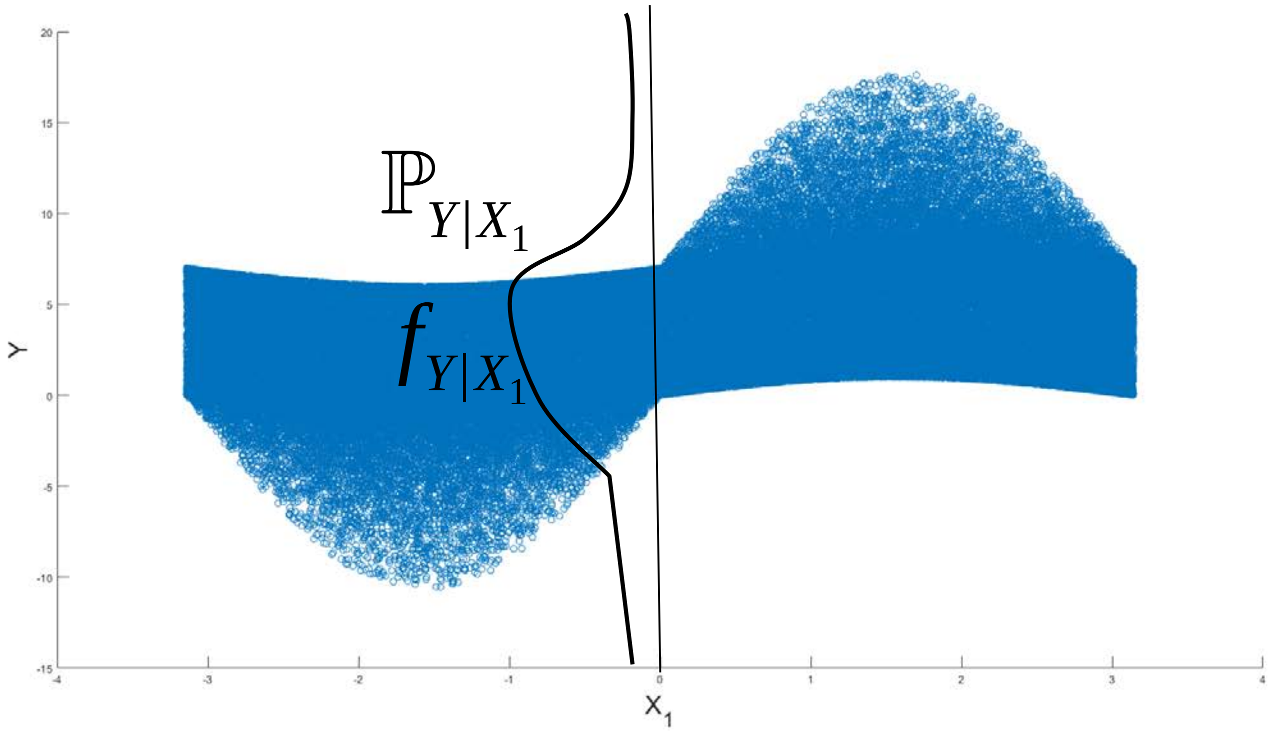
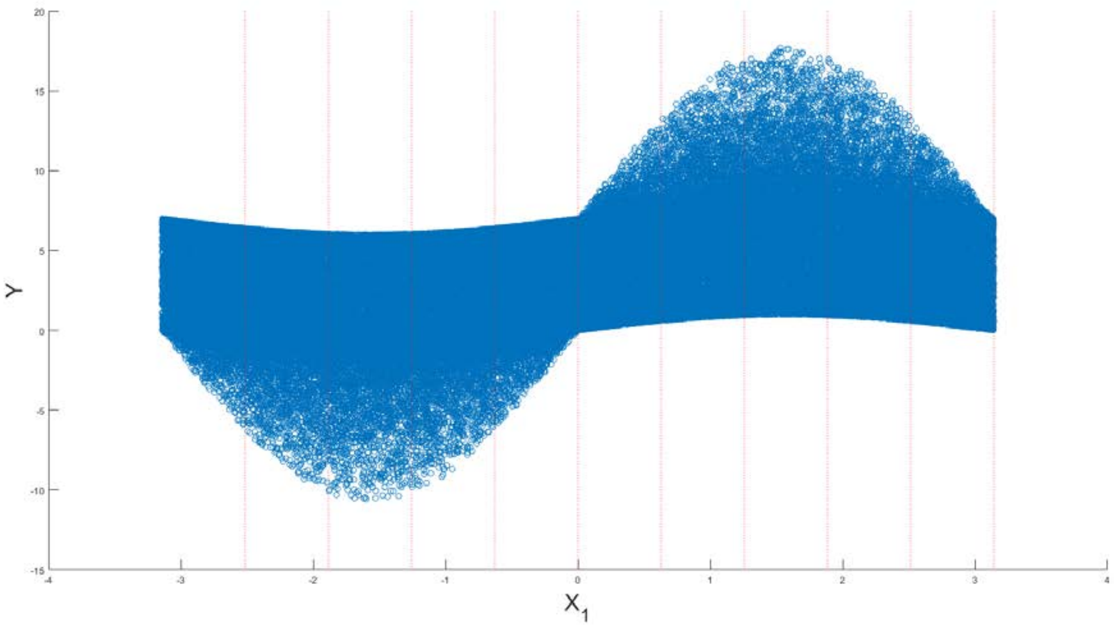
Ishigami Function Distribution



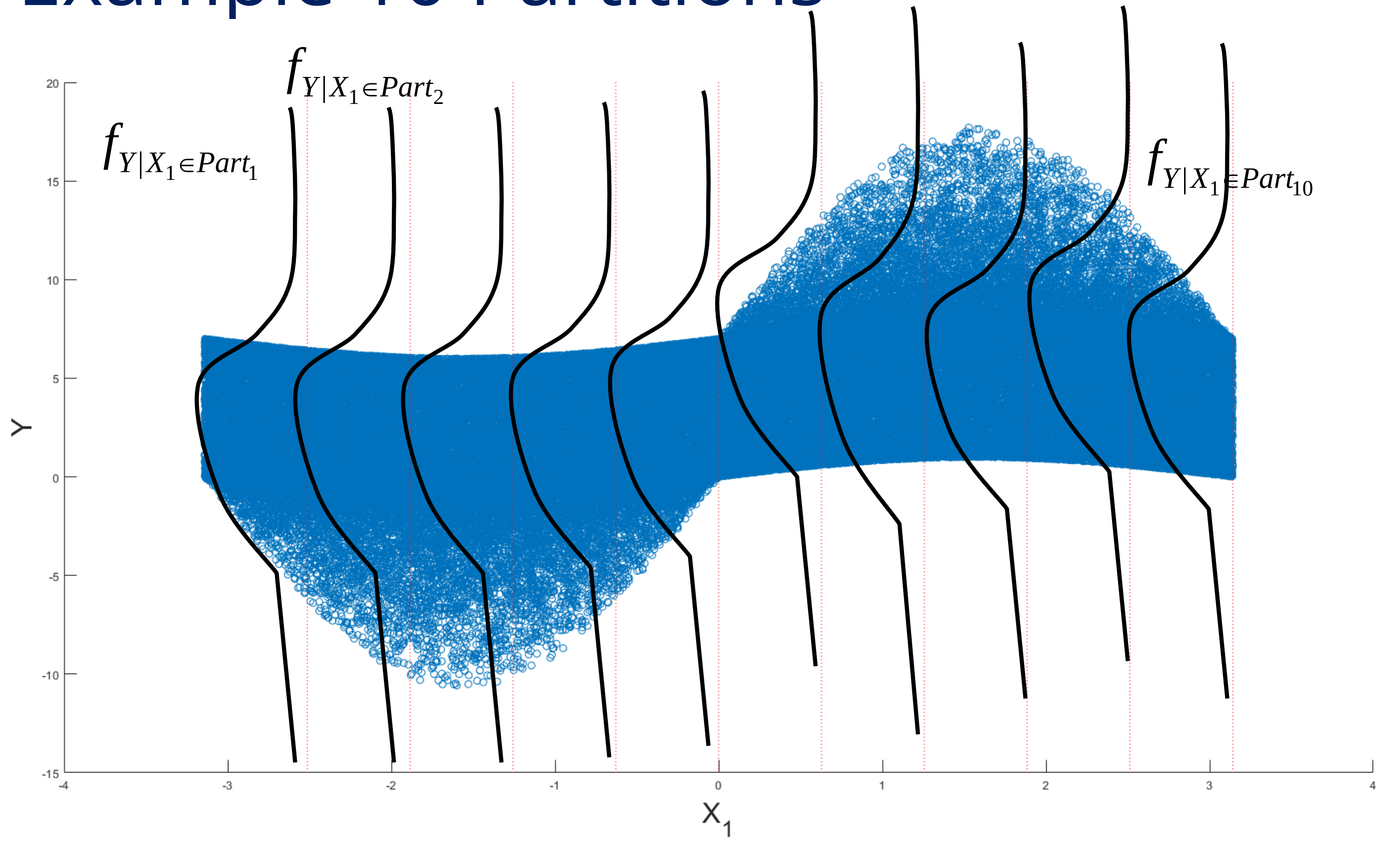
2) Form the scatterplot

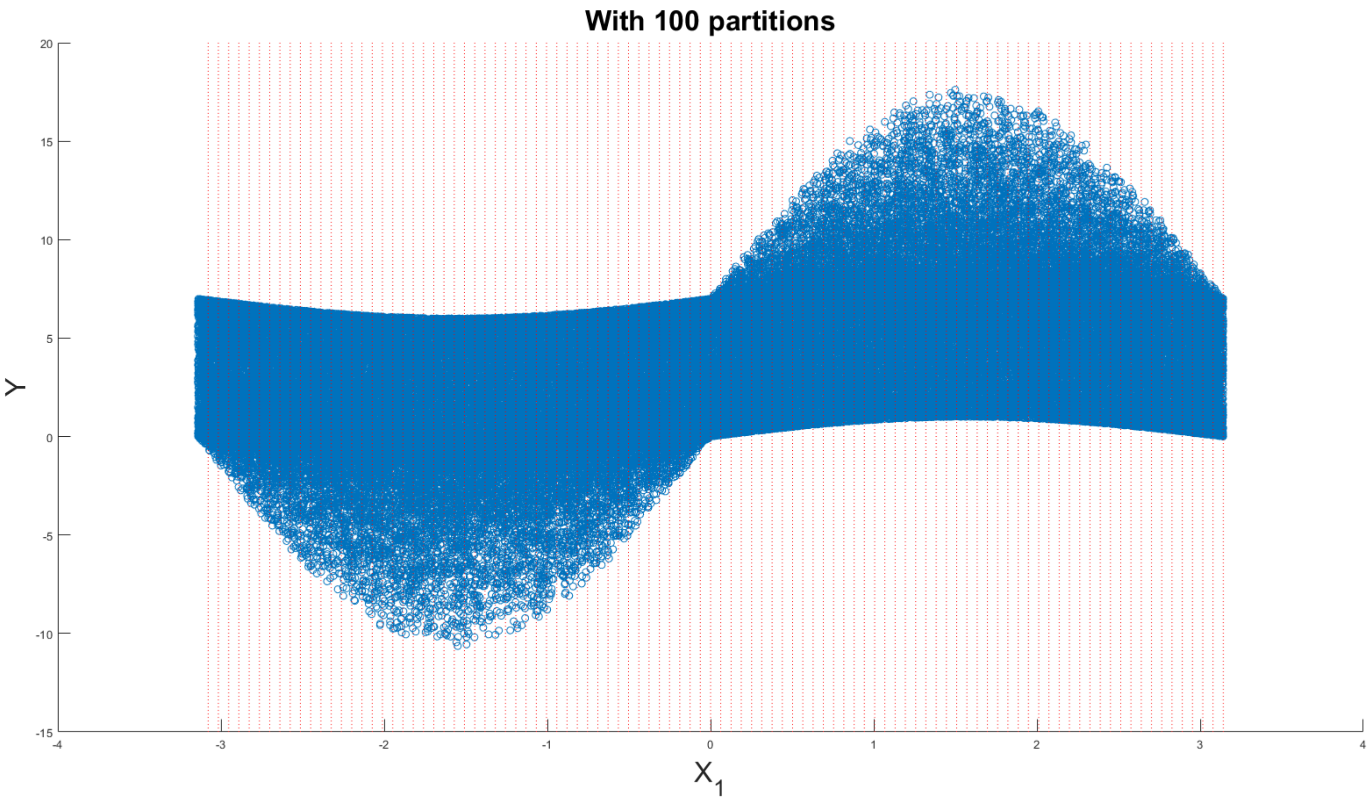


Partition the horizontal axis



3) Example 10 Partitions





With 100 partitions
Y
X1
20
15
10
5
0
-5
-10
-15
-4
-3
-2
-1
0
1
2
3
4

Given Data Estimation Theorem

1. *If* X *is finite then*

$$\lim_{N\to\infty} \xi_N^K = \xi^K(Y, X). \tag{44}$$

2. *In the general case, if* (42) *holds true,*

$$\lim_{M\to\infty} \lim_{N\to\infty} \xi_{M,N}^K = \xi^K(Y, X). \tag{45}$$

Experiments

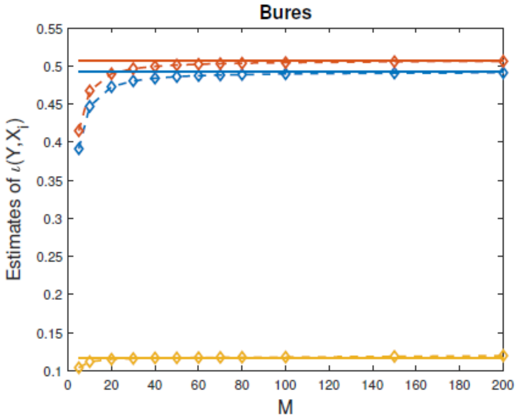


Figure 2: $\hat{\iota}(Y, X_i)$ for the multivariate-output analytical test case. The sample size is fixed at $N = 50000$. On the horizontal axis, partition cardinalities vary from $M = 5$ to $M = 200$.

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The Given Data OT-problem

Equation (46) implies the solution of an OT-problem for each of the M partitions. If the cost function is the squared Wasserstein metric, we need to solve:

$$\begin{gathered}\inf_{s} \sum_{k=1}^{N} \sum_{j: x_{j,i} \in \mathbb{X}_{\alpha}^{m}(N)} s_{k,j} \sum_{t=1}^{n_Y} (y_{k,t} - y_{j,t})^2 \\ \text{subject to} \\ \sum_{k=1}^{N} s_{k,j} = \frac{1}{N}, \sum_{j: x_{j,i} \in \mathbb{X}^{m}(N)} s_{k,j} = \frac{1}{N_m}, \quad N_m = \#\{j : x_{j,i} \in \mathbb{X}^{m}(N)\},\end{gathered} \tag{47}$$

Results for Alternative Solvers

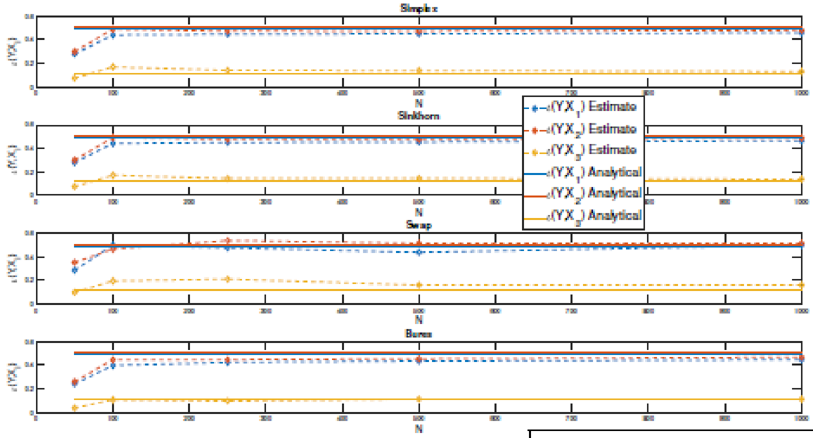
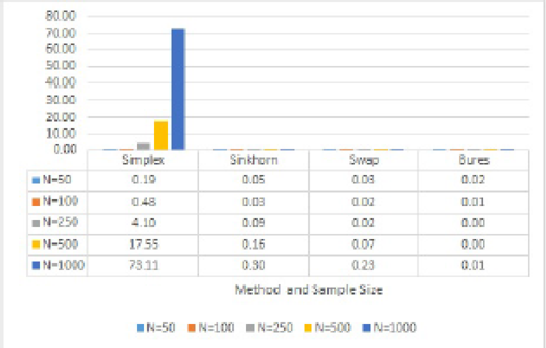


fig:MultivGaussTime

(a) $\hat{\iota}(Y, X_i)$



	Simplex	Sinkhorn	Swap	Bures
N=50	0.19	0.05	0.08	0.02
N=100	0.48	0.03	0.02	0.01
N=250	4.10	0.09	0.02	0.00
N=500	17.55	0.16	0.07	0.00
N=1000	73.11	0.30	0.23	0.01

(b) Times in seconds.

Figure 1: Estimates and times for experiments with sample sizes from $N = 50$ to $N = 1,000$ for four different algorithmic estimators of $\iota(Y, X_i)$ for the multivariate-output analytical test case used in this section.

Conclusions

- New Family of Indices for Multivariate Responses based on the theory of optimal transport
- Convenient Properties
- Generalize the previous multivariate indices of Lamboni (2011) and Gamboa et al (2014)
- Experiments Carried out thus far show promising results
- OT is a topical subject in AI, recent works propose breakthroughs in solution algorithms with interesting application perspectives