Variance reduction for estimation of Shapley effects and adaptation to unknown input distribution

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Framework and notation

- Random input vector $\boldsymbol{X} = (X_1, \dots, X_p)$ on space $\mathcal{X} = \mathcal{X}_1 \times \dots \times \mathcal{X}_p \subset \mathbb{R}^p$.
- $X_1, \dots, X_p$ are dependent.
- Deterministic black box function $f : \mathcal{X} \to \mathbb{R}$.
- Stochastic output

$$Y = f(\boldsymbol{X}).$$

- For $u \subseteq \{1, \dots, p\}$, let
  - $\boldsymbol{X}_u = (X_i, i \in u)$,
  - $-u = \{1, \dots, p\} \backslash u$,
  - $|u|$ be the cardinality of u.

Shapley effects

Conditional elements

For $u \subseteq \{1, \dots, p\}$, let

$$\mathrm{VE}_u = \mathrm{Var}\left(\mathbb{E}\left(Y|\boldsymbol{X}_u\right)\right)$$

and

$$\mathrm{EV}_u = \mathbb{E}\left(\mathrm{Var}\left(Y|\boldsymbol{X}_{-u}\right)\right).$$

Large VE_u or $\mathrm{EV}_u \Longrightarrow \boldsymbol{X}_u$ is important.

Shapley effects [Shapley, 1953, Owen, 2014, Iooss and Prieur, 2019]

For $i \in \{1, \dots, p\}$, the Shapley effect η_i is

$$\eta_i = \frac{1}{p\mathrm{Var}(Y)} \sum_{u \subset -\{i\}} \binom{p-1}{|u|}^{-1} \left(W_{u \cup \{i\}} - W_u\right),$$

with $W_u = \mathrm{VE}_u$ or $W_u = \mathrm{EV}_u$.

- $0 \leq \eta_i \leq 1$.
- $\sum_{i=1}^{p} \eta_i = 1$.
- Easy interpretation as percentage of importance even with dependent inputs.
- Even if f does not depend on variable i, we can have $\eta_i > 0$ if $\boldsymbol{X}_i$ is correlated with $\boldsymbol{X}_j$ and f depends on variable j.

Non-given data framework and double Monte Carlo

Non-given data framework

- We can choose any $\boldsymbol{x} \in \mathcal{X}$ and compute $f(\boldsymbol{x})$.
- We can sample from the conditional distributions of $\boldsymbol{X}$.

Estimation of EV_u by double Monte Carlo

Estimator

$$\widehat{\mathrm{EV}}_u = \frac{1}{N_u} \sum_{n=1}^{N_u} \frac{1}{N_I - 1} \sum_{k=1}^{N_I} \left(f\left(\boldsymbol{X}_{-u}^{(n)}, \boldsymbol{X}_u^{(n,k)}\right) - \overline{f\left(\boldsymbol{X}_{-u}^{(n)}\right)} \right)^2 .$$

- $\boldsymbol{X}_{-u}^{(1)}, \dots, \boldsymbol{X}_{-u}^{(N_u)}$ iid with law of $\boldsymbol{X}_{-u}$.
- $\boldsymbol{X}_u^{(n,1)}, \dots, \boldsymbol{X}_u^{(n,N_I)}$ iid with law of $\boldsymbol{X}_u$ conditionally to $\boldsymbol{X}_{-u}^{(n)}$.
- $\overline{f\left(\boldsymbol{X}_{-u}^{(n)}\right)}$ is the average of $f\left(\boldsymbol{X}_{-u}^{(n)}, \boldsymbol{X}_u^{(n,1)}\right), \dots, f\left(\boldsymbol{X}_{-u}^{(n)}, \boldsymbol{X}_u^{(n,N_I)}\right)$.

$\Longrightarrow$ Unbiased.
$\Longrightarrow$ We take $N_I = 3$ as in [Song et al., 2016].
$\Longrightarrow$ N_u is the budget/accuracy parameter.

Pick-freeze : an estimator of VE_u (not detailed explicitly here) [Janon et al., 2014].

Subset aggregation of estimators of conditional elements

- For $u \subseteq \{1, \ldots, p\}$, consider the estimator $\widehat{\mathrm{EV}}_u$ of EV_u.
- Then subset aggregation simply means summing over all subsets :

$$\widehat{\eta}_i = \frac{1}{p\widehat{\mathrm{Var}}(Y)} \sum_{u \subset -\{i\}} \binom{p-1}{|u|}^{-1} \left(\widehat{\mathrm{EV}}_{u \cup \{i\}} - \widehat{\mathrm{EV}}_u \right).$$

Question : For each $u \subseteq \{1, \ldots, p\}$, which budget (number of samples N_u) to allocate to $\widehat{\mathrm{EV}}_u$?

Contribution : optimal budget allocation

The optimal choice of $(N_u)_u$ subject to $\sum_{\substack{u \subseteq \{1,\ldots,p\} \\ u \neq \varnothing, \{1,\ldots,p\}}} N_u = N_{\mathrm{tot}}$ is

$$N_u^* \propto \sqrt{(p - |u|)!|u|!(p - |u| - 1)!(|u| - 1)!\mathrm{Var}(\widehat{\mathrm{EV}}_u^{(1)})},$$

with $\widehat{\mathrm{EV}}_u^{(1)}$ computed with budget $N_u = 1$.
$\Longrightarrow$ Issue : $\mathrm{Var}(\widehat{\mathrm{EV}}_u^{(1)})$ unknown.
$\Longrightarrow$ For practice (with some approximations) we take

$$N_u^* \propto \mathrm{Round}\left(\binom{p}{|u|}^{-1} \right).$$

Prospect : For large p, have $N_u^* = 0$ for many u to be computationally scalable ?

Random-permutation aggregation

- For a permutation σ on $\{1, \dots, p\}$ and $i \in \{1, \dots, p\}$, we let $P_i(\sigma) = \{\sigma(j);\ j = 1, \dots, \sigma^{-1}(i) - 1\}$. We have [Song et al., 2016]

$$\eta_i = \frac{1}{p!\mathrm{Var}(Y)} \sum_{\substack{\text{permutations} \\ \sigma}} (\mathrm{EV}_{P_i(\sigma) \cup \{i\}} - \mathrm{EV}_{P_i(\sigma)}).$$

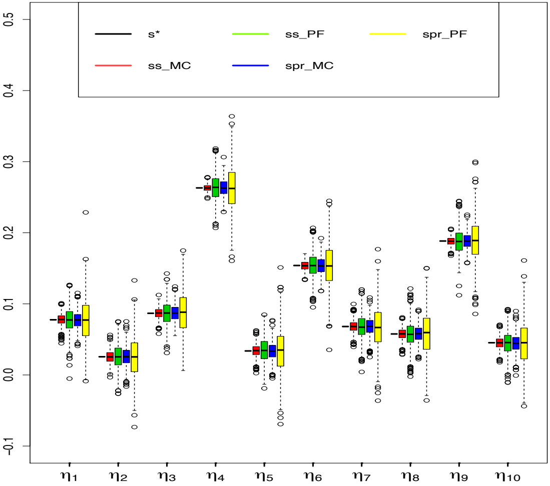
- Hence the random-permutation aggregation :

$$\widehat{\eta}_i = \frac{1}{\widehat{\mathrm{Var}}(Y)} \frac{1}{M} \sum_{j=1}^{M} (\widehat{\mathrm{EV}}_{P_i(\sigma_j) \cup \{i\}} - \widehat{\mathrm{EV}}_{P_i(\sigma_j)}),$$

  with $\sigma_1, \dots, \sigma_M$ iid random permutations (uniform).
- [Song et al., 2016] suggests to take the budget for each $\widehat{\mathrm{EV}}_u$ minimal ($N_u = 1$) and to take M maximal.

A Gaussian linear example.

- $s^\star$: true value.
- *ss* : subset aggregation.
- *spr* : random permutation.
- *MC* : double Monte Carlo for $\widehat{\mathrm{EV}}_u$.
- *PF* : pick-freeze for $\widehat{\mathrm{VE}}_u$.



1 Shapley effects

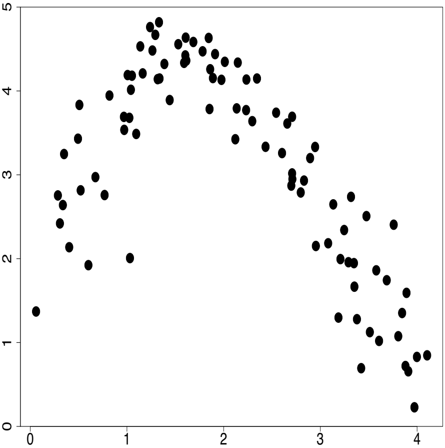
2 Improving estimation in non-given data framework

3 Given data framework with nearest-neighbors

Given data framework

- Only a data set of the input variables is available : $\boldsymbol{X}^{(1)}, \ldots, \boldsymbol{X}^{(n)}$ iid with the distribution of $\boldsymbol{X}$.
- The corresponding $Y_1 = f(\boldsymbol{X}^{(1)}), \ldots, Y_n = f(\boldsymbol{X}^{(n)})$ are available
  OR
  f can be called at any input $\boldsymbol{x}$.
- The exact conditional sampling needed by the previous estimators is not available.
- We will mimick this conditional sampling using nearest neighbors.

Nearest-neighbor approximation of conditional distributions



Estimator of EV_u with nearest-neighbors

- Recall
$$\mathrm{EV}_u = \mathbb{E}\left(\mathrm{Var}\left(Y|\boldsymbol{X}_{-u}\right)\right).$$
- Let $k_n^{-u}(i,\ell)$ be the ℓ-th nearest neighbor of $\boldsymbol{X}_{-u}^{(i)}$ among $\boldsymbol{X}_{-u}^{(1)}, \dots, \boldsymbol{X}_{-u}^{(n)}$.
- The estimator is

$$\begin{aligned}
\widehat{\mathrm{EV}}_u &= \frac{1}{n}\sum_{i=1}^{n}\frac{1}{N_I - 1}\sum_{\ell=1}^{N_I}\left(f\left(\boldsymbol{X}_{-u}^{(k_n^{-u}(i,\ell))}, \boldsymbol{X}_{u}^{(k_n^{-u}(i,\ell))}\right) - \overline{f\left(\boldsymbol{X}_{-u}^{(i)}\right)}\right)^2 \\
&= \frac{1}{n}\sum_{i=1}^{n}\frac{1}{N_I - 1}\sum_{\ell=1}^{N_I}\left(Y_{k_n^{-u}(i,\ell)} - \overline{Y_i}\right)^2
\end{aligned}$$

with

$$\overline{f\left(\boldsymbol{X}_{-u}^{(i)}\right)} = \text{ average}\left(f\left(\boldsymbol{X}_{-u}^{(k_n^{-u}(i,1))}, \boldsymbol{X}_{u}^{(k_n^{-u}(i,1))}\right), \dots, f\left(\boldsymbol{X}_{-u}^{(k_n^{-u}(i,N_I))}, \boldsymbol{X}_{u}^{(k_n^{-u}(i,N_I))}\right)\right)$$

$$\overline{Y_i} = \text{ average}\left(Y_{k_n^{-u}(i,1)}, \dots, Y_{k_n^{-u}(i,N_I)}\right).$$

- Other variants available when we can call $f(\boldsymbol{x})$ at new $\boldsymbol{x}$.
- This time, good choice of N_I is more open. Not necessarily $N_I = 3$.
- Similarities with rank methods for $|-u| = 1$ [Gamboa et al., 2020].

Rate of convergence

- Consider a fixed $u \subseteq \{1, \ldots, p\}$.

Condition

The function f is C^1, $\mathcal{X}$ is compact in $\mathbb{R}^p$, and $\boldsymbol{X}$ has a density $f_{\boldsymbol{X}}$ with respect to Lebesgue measure that is lower and upper bounded and Lipschitz continuous.

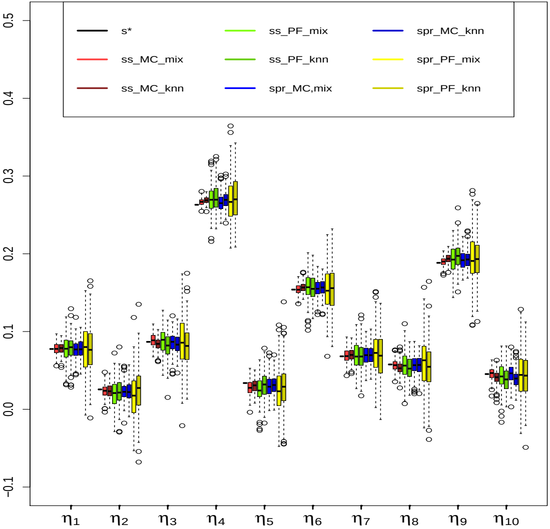
Contribution : rate of convergence

We have, for each $\delta > 0$,

$$\left| \widehat{\mathrm{EV}}_u - \mathrm{EV}_u \right| = o_p \left(\frac{1}{n^{\frac{1}{2(p-|u|)} - \delta}} \right).$$

- $p - |u| = |-u|$ is the dimension of the nearest-neighbor approximation $\Longrightarrow$ curse of dimensionality.
- When $p - |u| = 1$, essentially we reach parametric rate $n^{-1/2} \Longrightarrow$ optimal.
- For $p - |u| > 1$, is the rate optimal ?

- $s^{\star}$: true value.
- *ss* : subset aggregation.
- *spr* : random permutation.
- *MC* : double Monte Carlo for $\widehat{\mathrm{EV}}_u$.
- *PF* : pick-freeze for $\widehat{\mathrm{VE}}_u$.
- *knn* : nearest neighbor estimation.
- *mix* : a variant with new calls to f.



Conclusion

Conclusion :

- $\eta_1, \ldots, \eta_p$ are percentages of importance for dependent inputs.
- Estimation by aggregating $\widehat{\mathrm{EV}}_u$, $u \subseteq \{1, \ldots, p\}$.
- Can be beneficial to tune budgets N_u, $u \subseteq \{1, \ldots, p\}$.
- Nearest neighbors to mimick conditional distributions.

The paper :

B. Broto, F. Bachoc and M. Depecker, Variance reduction for estimation of Shapley effects and adaptation to unknown input distribution, *SIAM/ASA Journal on Uncertainty Quantification*,8(2) : 693–716, 2020

The R implementation : Function `shapleySubsetMC` in R package `sensitivity`.

Some follow-up works : [Broto et al., 2022, Demange-Chryst et al., 2022].

Many other ongoing work and prospects :

- Large dimension p, link with Hilbert-Schmidt Independence Criterion, interactions with machine learning...
- [Da Veiga, 2021, Ghorbani and Zou, 2019],...

Thank you for your attention !

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