Derivative-based upper bound for entropic total effect sensitivity with high dimensional and dependent inputs

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This research is motivated by applications of global sensitivity analysis (GSA) towards mathematical models of engineering problems. Such problems are common in computer experiments, where a physical phenomenon is studied with a complex numerical code, and GSA is employed to increase understanding of how the system works, reduce the problem's dimensionality, and help with calibration and verification. In this context, an important question for GSA is: 'Which model inputs can be fixed anywhere over its range of variability without affecting the output?'.

The most common GSA approach examines variability using the output variance. The variance-based total sensitivity indices provide the proportion of variance explained by the input variables. Such tools are limited to second-moment information, which presents a challenge if the underlying distribution is highly skewed or multi-modal. Entropy-based measures overcome this limitation, as they are applicable independent of the shape of the distribution. However, entropy-based indices have limited application in practice, mainly due to the heavy computational burden, as knowledge of conditional probability distributions is required.

In contrast, for a differentiable function, derivative-based methods can be more efficient. An inequality linking variance-based GSA and derivative-based measures has been established [1, 2] to detect un-influential input variables. A recent study [3] has proposed a derivative-based upper bound for entropy-based sensitivity indices, which is computationally cheap to estimate.

In this paper, we present a tighter entropic upper bound by including a differential mutual information correction that accounts for the impact of interactions between dependent input variables. We provide proof that for a differentiable deterministic function $y = g(\mathbf{x}) : R^d \to R$ with continuous random inputs, there exists an upper bound for the conditional entropy-based SA indices:

$$E[H(Y|\mathbf{X}_{\sim i})] \leq H(X_i) + l_i - I(X_i; \mathbf{X}_{\sim i}) \tag{1}$$

where $\sim i$ indicates the index ranges from 1 to d excluding i. $H(X_i)$ is the differential entropy of the input variable X_i and l_i is the expected log-derivatives $l_i = E\left[\ln |\partial g(\mathbf{x})/\partial x_i|\right]$. The mutual information $I(\cdot\,;\cdot)$ is a moment-independent quantification of the statistical dependence between variables reflecting their amount of shared information. As the mutual information is nonnegative, the new upper bound is tight when dependencies among input variables are known or suspected. This greatly improves the screening power, as the effectiveness of the screening improves with the tightness of the upper bound.

Another issue for the derivative-based upper bound is the lack of verification for high-dimensional problems. The simulation of differential entropy, mutual information, and related information theoretic quantities typically proceeds using 'plug-in' Monte Carlo estimators where the densities required are approximated using nonparametric kernel density estimation techniques. However, it is well-known that even in dimensions as low as 10, kernel density estimation is prohibitively data-inefficient [4].

To overcome this issue, we utilize neural density estimation techniques, including recent algorithmic advancements such as MINE [5], KNIFE [6], and REMEDI [7], for efficient approximation of information-theoretic quantities in high dimensions. These estimators are differentiable with respect to the data, enabling the global sensitivity measures to be optimized for outer-loop tasks in engineering design.

Simulation-based prototyping for engineering design problems often involves high-dimensional spaces of possibly correlated and dependent control variables. This paper extends the derivative-based entropic upper bound to high-dimensional and dependent inputs, thus providing a versatile and efficient tool for general engineering applications.

Reference

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