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AN EFFECTIVE PARAMETER SCREENING STRATEGY FOR HIGH DIMENSIONAL MODELS

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ABSTRACT

The method of Elementary Effects (EE) is a parameter screening type sensitivity analysis technique that combines advantages of inexpensive one-at-a time methods and expensive variance decomposition based global Sensitivity Analysis (SA) techniques. Most of the sampling strategies for EE either use random sampling or maximize sample spread through oversampling. The Sampling for Uniformity (SU) is the only available strategy that combines the principle of sample spread with the principle of uniformity.

In this work, we proposed modifications to SU (eSU) to further improve sample uniformity. Performance of eSU was compared to that of SU based on uniformity, sample spread, sample generation time, and screening efficiency. Importance of the concept of uniformity was strengthened as eSU outperformed SU across all evaluation criteria. Further, it was found that eSU does not need oversampling and can result in better screening with relatively few trajectories indicating significantly reduced requirement on computational resources.

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NOMENCLATURE

T_{μ^*}	set of important parameters identified from EE exercise based on μ^*
T_{ST}	set of truly important parameters
$Time^Q$	Sample generation time normalized with respect to that of Q = 1
$Time^r$	Sample generation time normalized with respect to that of r = 4, Q = 1
gST	screening efficiency
gST^Q	screening efficiency normalized with respect to that of Q = 1
k	number of parameters
q	number of parameter levels
Q	oversampling size
r	number of trajectories
Δ	parameter perturbation size in unit hyperspace
μ_i^*	mean of absolute values of elementary effects associated with i^{th} parameter
μ_i	mean of elementary effects associated with i^{th} parameter
σ_i	standard deviation of elementary effects associated with i^{th} parameter

INTRODUCTION

Sensitivity analysis (SA) is an extremely useful model evaluation technique that can serve many purposes such as model corroboration, parameter identification, research prioritization, model based decision making, and others [1,2]. Large scale system models such as climate models, environmental flow models, building energy models are characteristically high-dimensional, complex in nature and often require substantial simulation time. This large dimensionality poses numerous challenges in terms of computational resources on more rigorous SA techniques such as Sobol' analysis [3-5]. Due to this, the Elementary Effects (EE) method [6] has received considerable attention during the last decade as it can perform Global Sensitivity Analysis (GSA) at an exceptionally low computational cost, though relatively qualitatively [7,8]. Several studies have recommended incorporation of the EE technique as an essential step to identify important parameters before implementing more rigorous model analysis (e.g., [9]). In some cases, modelers have relied solely on EE analysis (e.g., [10-12]) or used EE analysis to replace traditional design of experiments for laboratory studies [13].

The downside of the low computational cost of EE analysis is that the sample is a relatively sparse representation of the parameter space which can have substantial effect on screening performance. This has been the motivation behind the refinement of parameter sampling in EE analysis as evident from the development of as many as eleven different sampling strategies between 2006 and 2016 (Table 1). Note that these strategies vary in terms of sampling principles (*e.g.*, (a) sample spread: Optimized Trajectories [OT], Modified Optimized Trajectories [MOT], Quasi OT [QOT], (b) local polytopes: Latin Hypercube One-at-a-Time, Simplex, Constellations, and others) and other characteristics (fixed step or variable step, winding stairs or radial trajectories, *etc*.). Literature survey indicates that fixed step trajectory-based sampling strategies are more popular among modelers.

Khare *et al*. (2015) developed a trajectory-based sampling strategy – Sampling for Uniformity (SU) based on the dual principle of (a) uniformity and (b) spread. Their results pointed that sample spread does not play as important a role in enhancing screening efficiency of EE analysis as initially thought. A typical way of obtaining optimal sample spread, *i.e.,* hyper distance between trajectories, is through oversampling. In OT and MOT (Table 1) oversampling refers to generating very large pool of parameter trajectories from which a final smaller sample is chosen while in SU it implies generating the entire parameter sample multiple times. Sample spread maximization algorithms in purely spread based techniques such as OT and MOT can make them impractically time consuming, especially in high-dimensional problems at recommended oversampling sizes, which was also noted by [15]. On the other hand, [14] concluded that improved sample uniformity in SU helped in producing better and stable parameter screening across a range of benchmark functions at just a fraction of the sample generation time of OT and MOT. Though SU was not the first strategy to recognize the importance of uniformity, it was the first one to explicitly use it as its sampling basis.

Fixed grid trajectory based sampling for the method of EE assumes that all parameters follow discrete uniform distributions in unit parameter hyperspace [6]. The uniformity algorithm used in SU aimed at generating samples such that parameter distributions were discrete uniform for only the first and the last points of the trajectories. While this helped in improving the overall uniformity of the sample, it does not ensure or imply complete uniformity considering all sample points *i.e.,* complete uniformity. This point continues to be a matter of concern since complete uniformity is a critical requirement of EE.

OBJECTIVES

The objective of this work was to modify SU to enhance the uniformity considering all sample points with the aim of improving screening efficiency without adversely impacting the time required for sample generation. The modified SU or enhanced SU (eSU), formulated by making changes to SU, was then compared to the original SU on the basis of uniformity, sample spread, sampling time, and screening efficiency. For the screening efficiency, a suite of six benchmark test functions was used. Since computational time and screening performance are affected by oversampling size (Q) and number of trajectories (r), SU *vs*. eSU comparison was extended to study these effects to identify ideal sampling settings for these techniques.

ELEMENTARY EFFECTS METHOD

The method of Elementary Effects (EE) or EE method [6] is a low-cost GSA technique typically used in parameter screening type of experiments. Sample consists of r trajectories each of (k+1) points such that from every trajectory k numerical derivatives (Elementary Effects), one corresponding to each parameter (model dimension) are calculated (Eq. (1)). The r trajectories give r EEs from the entire sample which are then statistically analyzed to estimate two sensitivity measures, μ_i and σ_i (Eq. (2a) and Eq. (3)). Measure μ_i was later modified to use the absolute value of the elementary effects, μ_i^* (Eq. (2b)) to make it suitable also for non-monotonic outputs [16].

$$EE_i = \frac{y(p1,p2,\ldots,pi+\Delta,\ldots,pk)-y(p1,p2,\ldots,pi,\ldots,pk)}{\Delta} \tag{1}$$

$$\mu_i = \frac{1}{r}\sum_{j=1}^{r} EE_i^j \tag{2a}$$

$$\mu_i^* = \frac{1}{r}\sum_{j=1}^{r} |EE_i^j| \tag{2b}$$

$$\sigma_i = \sqrt{\frac{1}{r}\sum_{j=1}^{r}(EE_i^j - \mu_i)} \tag{3}$$

where y = model, while p1, p2... pk = model parameters.

Parameters are plotted in μ* - σ space to identify model behavior related to them and to segregate them into important and unimportant classes as schematically shown in Fig. 1. It has been empirically shown that μ* is equivalent of total effect sensitivity index calculated in variance decomposition based GSA techniques and is primarily used for parameter ranking/screening [16]. The total computational cost associated with EE method is r(k+1). Typically, r is chosen in the range of 10-30. However, in the literature there is no consensus with different studies recommending from as few as 2 to as many as over 100 trajectories (*e.g.,* [17-19]) without formally analyzing an ideal number for r across a range of functions.

SAMPLING PROCEDURE: SU AND eSU

Sampling for Uniformity (SU) is a trajectory based sampling scheme which uses a fixed grid to generate samples [14]. Fixed grid implies that each parameter can take only q values. EE sampling methods literature indicates that q is commonly set at 4. Figure 2a schematically shows the three-step sampling procedure of SU. In the first step the first and the last points of all trajectories are sampled such that each level is sampled evenly for each of the parameters and the points are unique. The second step consists of randomly generating a unique perturbation vector for each trajectory so that the sample is unique. In the third step, steps 1 and 2 are repeated Q times and the trajectory set for which the spread is highest is selected as the final sample.

In eSU, modifications were made to step 2 of SU (Fig. 2b). Instead of generating a separate perturbation vector for each trajectory, a fixed perturbation vector was proposed for all trajectories. Elements of this fixed vector are {1, 2, 3, 4, …, k-1}. In other words, for all trajectories parameter coordinates are changed sequentially from 1 to k to form the remaining trajectory points. That is, the second point is formed by changing the first parameter coordinate of the first point, the third point is formed by changing the second parameter coordinate of the second point and so on (see Fig. 3).

Two sets of numerical experiments were conducted to compare SU and eSU. The first targeted solely towards testing the efficacy of modifications to SU algorithm for uniformity enhancement. Following settings were used in these uniformity experiments.

k = {10, 15, 20, 25, 30},
r = {6, 8, 10,12}, Q = {300},
Sampling Strategies = {SU, eSU}

The uniformity of the generated samples, considering all sample points, was evaluated through
(1) statistical testing using the Chi-square goodness of fit test for discrete uniform distribution at 5% significance level, and
(2) exact match between generated and theoretical distributions.

A second set of numerical experiments was conducted with the following settings to test impacts of Q and r on the overall efficiency of SU and eSU sampling in EE method (*i.e.,* sampling and screening) considering: (a) Euclidian Distance (ED), (b) screening efficiency, and (c) sample generation time under following setting.

k = {10, 15, 20},
r = {4, 8, 20, 40},
Q = {1,10,30,50,100,300,500,1000},
q = 4,
Sampling Strategies = {SU, eSU},
Test Functions = {K10, O15, M20, B20, G20, GS20}

Note that all experiments were repeated 100 times.

Euclidean Distance (ED) has been used as a standard measure for the spread of sample points in the parameter hyperspace in OT, MOT, SU and QOT. We visually compared ED obtained for SU and eSU for all combinations of Q-r-k. For a given sample, first the distance between any two sample trajectories 'a' and 'b' is calculated (Eq. (4)) to obtain distance matrix of size r * r. Distances in this matrix are geometrically summed (Eq. (5)) to calculate ED of the sample.

$$d_{a,b} = \sum_{i=1}^{k+1} \sum_{j=1}^{k+1} \sqrt{\sum_{z=1}^{k} [X_i^a(z) - X_j^b(z)]^2} \tag{4}$$

$$ED = \sqrt{\sum_{i=1}^{r} \sum_{j=1}^{r} d_{i,j}^2} \tag{5}$$

Sample generation time, on a given machine, for a specific dimensionality is affected by Q, r, and optimization scheme for ED/sampling strategy. To compare relative time efficiency of eSU with respect to SU, ratio of corresponding sample generation time for each combination of Q-r-k was calculated. As presented later, it was clear that eSU requires less computation time. Hence, effects of Q-r were analyzed for eSU alone. To study the impact of Q on time, raw time values were normalized as $Time^Q$ using Eq. (6)

$$Time^{\,Q} = \frac{time(eSU,r,Q,k)}{time(eSU,r,Q=1,k)} \tag{6}$$

On the other hand, effect of r on time was studied by calculating $Time^r$ using Eq. (7)

$$Time^{r} = \frac{time(eSU,r,Q,k)}{time(eSU,r=4,Q=1,k)} \tag{7}$$

The last evaluation criteria used in this study is the parameter screening efficiency, defined as the skill score gST, the ratio of the number of important parameters correctly identified by EE analysis to the number of important parameters (Eq. (8)).

$$gST = \frac{Count(T_{\mu*} \cap T_{ST})}{Count(T_{ST})} \tag{8}$$

This screening efficiency concept was also used in other works [14,17,20] to assess the impact of sampling strategies on parameter screening. As noted earlier, sensitivity measure μ* is equivalent to the total effect sensitivity index from variance-based GSA, making usage of gST justifiable.

For all six test functions (K10, O15, B20, G20, GS20, and M20) used in this screening efficiency study, important parameters can be identified through analytical expressions or are known from the literature. The number following the function indicates the dimensionality of the corresponding test functions. For example, B20 means that test function is B and it has 20 parameters. Details of these functions are given in the Appendix A.

gST can range between 0 and 1, with 1 being the perfect screening. Unlike sampling time, gST is not affected by machine used for computations or by dimensionality of the model. The only factors affecting it are Q, r, and sampling scheme. To study the effect of Q on gST we further normalized gST scores (gST^Q) by corresponding gST for eSU at Q = 1 as shown in Eq. (9). Note that gST^Q can be greater than 1. gST^Q results were plotted for all r-test function sampling strategy combinations.

$$gST^{\,Q} = \frac{gST(SS,r,Q,fun)}{gST(eSU,r,Q=1,fun)} \qquad (9)$$

where, SS = sampling strategy (SU or eSU); fun = test function.

Effect of r on gST was studied by plotting gST averaged over all Q values for each of the six test functions (Table 2 and Table 3). This was possible because for any given function, variation of gST with Q was found to be minimal and without any increasing trend.

RESULTS

Uniformity

The average fraction of parameters passing the Chi-square goodness of fit tests for the discrete uniform distribution are presented in Table 2. It can be observed that for all combinations of r–k–sampling strategy, uniformity deteriorated with increasing k, except for r = 8 and 12 in the case of eSU (where there were no failures *i.e.,* samples were perfectly uniform). For SU uniformity improved with increase in r (for any given k). Overall for any given r-k combination eSU samples were more uniform compared to SU samples and the rate of uniformity deterioration was smaller.

When the uniformity was tested using a different criterion (average fraction of parameters with a perfect discrete uniform distribution), it was observed that samples were far away from being perfectly uniform for all r–k combinations for SU (Table 3).

On the other hand, in the case of eSU samples were perfectly uniform irrespective of k for r = 8 and 12.

Euclidean Distance (ED)

Figure 4 shows ED plotted against Q for various k (10, 15 and 20) for r = 8. For all three model dimensionalities, ED between trajectories for eSU was higher than that of SU. Also, ED for eSU did not show much variation with Q. In the case of SU, ED values somewhat increased, however this trend was marked by considerable fluctuations. Similar results were observed for other k-r combinations. Importantly, eSU produced better and stable sample spread regardless of the oversampling size.

Sample Generation Time

Table 4 summarizes the time requirement of eSU sampling relative to SU. The sampling time ratio was found to be less than 1 irrespective of Q-r-k combinations. The ratio varied between 0.73 and 0.97, indicating eSU marginally reduced sampling time with respect to SU. This study considered dimensionalities only up to 20. Since in higher dimensions (often the case with complex models) sampling time can be of the order of days, even this marginal time improvement can prove to be beneficial [21].

Effect of Q and r on Sample Generation Time

Normalized sample generation time $Time^Q$ was plotted against Q for each combination of k-r used in numerical experiments. Figure 5 shows results for k = 15 and r = 8. It can be observed that $Time^Q$ increased linearly with Q. Note that $Time^Q$ *vs*. Q plots for other k-r combinations were identical to Fig. 5. Figure 6 shows plots of normalized sample generation time ($Time^r$) against r for all values of Q considered in numerical experiments for k = 15. For each Q, $Time^r$ followed power law, $Time^r = a\ r^b$, with b varying in a narrow range of 1.58 to1.6. $Time^r$-r relationships for k = 10 and 20 are not presented here for the sake of convenience. However, results were similar to those for k = 15. These $Time^r$ results indicate sample generation time increases very rapidly with r.

Screening Efficiency

The main purpose of any EE exercise is to identify important model parameters which makes screening efficiency the most important evaluation criteria used in this study. We studied effects of both the ingredients of sample size, *i.e.,* r and Q on gST. Since the interest was in identifying relative efficiency of eSU against SU, appropriate normalizations were applied to raw gST scores to segregate corresponding effects.

Effect of Q on Screening Efficiency

The relative normalized skill score gST^Q was plotted against Q for each test function for both SU and eSU at different values of r as shown in Fig. 7. Each row of subplots corresponds to one test function, while each column corresponds to one r value. Each subplot has two lines: solid line for eSU and dotted line for SU. It can be observed that irrespective of the test function, eSU performed better screening as SU curves were always lower or overlapping with eSU curves. Surprisingly, neither eSU nor SU showed improvement in gST^Q scores with respect to Q for any test function at any r.

The vertical differences between SU and eSU curves varied from function to function. For example, in case of M20 SU and eSU curves very much overlapped, while for O15 and G20 they remained well separated. For remaining functions, *i.e.,* K10, B20, and GS20 relative performances were strongly affected by r as vertical differences between SU and eSU curves distinctively diminished at higher r.

Effect of r on Screening Efficiency

To explicitly evaluate effect of r on gST, gST scores averaged over all Q values were plotted along with corresponding standard deviations as error bars as shown in Fig. 8. Both SU (dotted lines) and eSU (solid lines) showed saturation curve type behavior with respect to r. For all six functions eSU had higher (or same) gST score compared to SU, irrespective of r. Also, error bars for eSU were smaller than those of SU indicating that eSU results in more stable screening. The vertical separation between SU and eSU curves varied from function to function. For K10, B20, and GS20 functions the two curves came closer with increasing r while in O15 and G20 the behavior was opposite.

DISCUSSION

Sampling for EE experiments is constrained by many aspects such as sample size (number of trajectories), computational time requirements, and other sampling concepts like sample spread and uniformity. This multi-faceted nature of the problem has driven EE sampling research in different directions. In this study, our focus was to verify finding of [14] that sample uniformity plays extremely important role in the successful application of EE method, through the development of eSU algorithm. At the same time, attempts were made to put light on optimal sampling setting for the proposed method. To emphasize, EE sampling being a multi-faceted problem one needs to look at all possible aspects simultaneously to draw any concrete conclusions.

The uniformity results indicated that the new algorithm for the perturbation vector enhanced uniformity of SU. Interestingly in the SU – eSU comparison, perfect sample uniformity was achieved only for eSU when r = 8 and 12. Note that in this study q = 4 was used. Based on this we hypothesize that eSU generates perfectly uniform samples when r is a multiple of q. Values of r used in second set of experiments were selected based on this. With these perfect uniformity settings, in second set of experiments, eSU was found to produce higher EDs compared to SU along with higher gST score across suite of 6 test functions. Also, effect of Q on ED and gST was found to be minimal. Again, we can attribute this to the improved uniformity of eSU. These findings also imply that oversampling is not necessary for eSU. Since oversampling has been the main reason of excessive sample generation time requirements, 'no oversampling necessary' finding for eSU is a significant breakthrough.

Results of gST variation with r indicated that ideal sample size (*i.e.*, number of trajectories necessary for robust screening) depends on characteristics of model/function under consideration. Yet, for the suite of 6 test functions eSU could correctly screen 96% and 98% of parameters with r = 8 and 20, respectively.

On the other hand, r = 40 was not able to produce 100% accurate screening, implying that increasing number of trajectories may not guarantee accurate screening due to the asymptotic behavior of gST vs. r curve. Based on these results, an initial recommendation of r between 8 and 20 can be made for screening type of EE applications. These findings need to be further studied by analyzing a wider range of test functions.

SUMMARY

The algorithm for the perturbation vector in the sampling strategy of SU for the screening method of EE was modified with the aim of enhancing uniformity of generated samples. This modified version of SU called eSU indeed enhanced sample uniformity along with substantial improvement in screening efficiency without adversely affecting the computational demand. Rather, it was found that oversampling is not necessary in the case of eSU paving the way for substantially reducing sample generation time. Overall, eSU outperformed SU across all four (uniformity, parameter spread, sampling time and screening efficiency) evaluation criteria. We attribute superior performance of eSU to its ability to produce perfectly uniform samples with larger sample spread without oversampling when the number of trajectories is a multiple of number of parameter levels. Pending further investigation, it is recommended to use 8 to 20 trajectories for eSU when it is used in EE screening exercises. MATLAB implementation of eSU is available for free download from http://abe.ufl.edu/carpena/software/SUMorris.shtml.

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REFERENCES

[1] Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Galtelli, D., Saisana, M., and Tarantola, S., 2008. "*Global Sensitivity Analysis: The Primer*," Chichester, U.K., John Wiley and Sons, ISBN-978047005997.

[2] Borgonovo, E., 2017. "*Sensitivity Analysis: An Introduction for the Management Scientist*," ISBN 978-3-319-52259-3.

[3] Saltelli, A., Ratto, M. Tarantola, S. and F. Campolongo, F., 2005. "Sensitivity analysis for chemical models", *Chemical Reviews*, 105(7): 2811-2827.

[4] Tian, W., 2013. "A review of sensitivity analysis methods in building energy analysis," *Renewable and Sustainable*

Energy Reviews, 20, 411-419. https://doi.org/10.1016/j.rser.2012.12.014

[5] Menberg, K., Heo, Y., and Choudhary, R., 2016. "Sensitivity analysis methods for building energy models: Comparing computational costs and extractable information," *Energy and Buildings*, 133, 433-445.

[6] Morris, M.D., 1991. "Factorial sampling plans for preliminary computational experiments," *Technometric,* 33(2): 161-174.

[7] Vu-Bac, N., Lahmer, T., Keitel, H., Zhao, J., Zhuang, X., and Rabczuk, T., 2014. "Stochastic predictions of bulk properties of amorphous polyethylene based on molecular dynamics simulations," *Mechanics of Materials*, 68, 70-84.

[8] Picchi, D. and Poesio, P., 2017. "Uncertainty quantification and global sensitivity analysis of mechanistic one-dimensional models and flow pattern transition boundaries predictions for two-phase pipe flows," *International Journal of Multiphase Flow*, 90, 64-78.

[9] Garcia Sanchez, D., Lacarrière, B., Musy, M., and Bourges, B., 2014. "Application of sensitivity analysis in building energy simulations: Combining first-and second-order elementary effects methods," *Energy and Buildings,* 68, 741-750.

[10] Shen, Z., Hong, Q., Yu, H., and Liu, R., 2008. "Parameter uncertainty analysis of the non-point source pollution in the Danning River watershed of the Three Gorges Reservoir Region, China," *Science of Total Environment* 405: 195-205.

[11] Srivastava, V., Graham, W.D., Muñoz-Carpena, R., and Maxwell, R.M., 2014. "Insights on geologic and vegetative control over hydrologic behavior of a large complex basin – Global Sensitivity Analysis of an integrated parallel hydrologic model," *Journal of Hydrology* 519: 2238-2257. doi: 10.1016/j.jhydrol.2014.10.020.

[12] Fezi, K. and Krane, M.J.M., 2017. "Uncertainty quantification in modelling equiaxed alloy solidification," *International Journal of Cast Metals Research*, 30(1), 34-49.

[13] Rodea-Palomares, I., Gonáalez-Pleiter, M., Gonzalo, S., Rosal, R., Leganés, F., Casellas, M., Muñoz-Carpena, R., and Fernandez-Piñas, F., 2016. "Hidden drivers of low-dose pharmaceutical pollutant mixtures revealed by the novel GSA-QHTS screening method," *Science Advances (AAAS)* 2(9):e1601272. doi: 10.1126/sciadv.1601272.

[14] Khare, Y.P., Muñoz-Carpena, R., Rooney, R., and Martinez, C.J., 2015. "A multi-criteria trajectory-based parameter sampling strategy for the screening method of elementary effects," *Environmental Modelling and Software* 64: 230-239. doi.org/10.1016/j.envsoft.2014.11.013.

[15] Ge, Q., Ciuffo, B., and Menendez, M., 2015. "Combining screening and metamodel-based methods: an efficient sequential approach for the sensitivity analysis of model outputs," *Reliability Engineering and System Safety* 134: 334-344. doi:10.1016/j.ress.2014.08.009

[16] Campolongo, F., Cariboni, J. and Saltelli, A., 2007. "An effective screening design for sensitivity analysis of large models," *Environmental Modelling and Software* 22: 1509-1518. doi:10.1016/j.envsoft.2006.10.004

[17] Campolongo, F., Saltelli, A. and Cariboni, J., 2011. "From screening to qualitative sensitivity analysis. A unified approach," *Computer Physics Communications* 182: 978-988. doi:10.1016/j.cpc.2010.12.039

[18] Herman, J.D., Kollat, J.B., Reed, P.M., and Wagener, T., 2013. "From maps to movies: high resolution time-varying sensitivity analysis for spatially distributed watershed model", *Hydrology Earth System Science* 17: 5109-5126. doi: 10.5194/hess-17-5109-2013

[19] Wainwright, H.M., Finsterle, S., Jung, Y., Zhou, Q. and Birkholzer, J.T., 2014. "Making sense of global sensitivity analyses", *Computers and Geosciences* 65: 84-94.

[20] Xiao, S., Lu, Z., and Xu, L., 2016. "A new effective screening design for structural sensitivity analysis of failure probability with the epistemic uncertainty", *Reliability Engineering & System Safety, 156,* 1-14.

[21] Khare, Y.P., 2014. "Hydrologic and water quality model evaluation with global sensitivity analysis: Improvements and applications," Ph.D. Dissertation, Department of Agricultural and Biological Engineering, University of Florida, Gainesville, Florida, U.S.A..

[22] Sobol, I.M., 1993. "Sensitivity analysis for non-linear mathematical models," *Mathematical Modelling and Computer Experiments* 1: 407-414.

[23] Saltelli, A. and Sobol, I.M., 1995. "About the use of rank transformation in sensitivity analysis of model output," Reli*ability Engineering and System Safety* 50: 225-239.

[24] Saltelli, A. and Annoni, P., 2010. "How to avoid a perfunctory sensitivity analysis", *Environmental Modelling and Software* 25: 1508-1517. doi: 10.1016/j.envsoft.2010.04.012

[25] Saltelli, A., Annoni, P., Azzini, I., Campolongo, F., Ratto, M., and Tarantola, S., 2010. "Variance based sensitivity analysis of model output. Design and estimator for total sensitivity index," *Computer Physics Communications* 181: 259-270.

[26] van Griensven, A., Meixner, T., Grunwald, S., Bishop, T., Diluzio, M., and Srinivasan, R., 2006. "A global sensitivity analysis tool for the parameters of multi□ variable catchment models," *Journal of Hydrology* 324(1–4): 10–23.

[27] Pujol, G., 2009. "Simplex based screening designs for estimating metamodels," *Reliability Engineering and System Safety* 94: 1156-1160.

[28] Saltelli, A., Campolongo, F., and Cariboni, J., 2009. "Screening important inputs in models with strong interaction properties," *Reliability Engineering and System Safety* 94: 1149-1155. doi:10.1016/j.ress.2008.10.007

[29] Ruano, M.V, Ribes, J., Seco, A., and Ferrer, J., 2012. "An improved sampling strategy based on trajectory design for application of the Morris method to systems with many input factors," *Environmental Modelling and Software* 37: 103-109.
[30] Santiago, J., Corre, B., Claeys-Bruno, M., and Sergent, M., 2012. "Improved sensitivity through Morris extension," *Chemometrics and Intelligent Laboratory Systems* 113:52-57. doi: 10.1016/j.chemolab.201110.006.
[31] Oakley, J.E. and O'Hagan, A., 2004. Probabilistic sensitivity analysis of complex models: A Bayesian approach. Journal of the Royal Statistical Society Series B 66: 751-769. doi: 10.1111/j.1467-9868.2004.05304.x
[32] Loubière, P., Jourdan, A., Siarry, P., and Chelouah, R., 2016. "A sensitivity analysis method for driving the Artificial Bee Colony algorithm's search process," *Applied Soft Computing* 41: 515-531. doi.org/10.1016/j.asoc.2015.12.044

APPENDIX A

TEST FUNCTIONS

Details of test functions and the sets of important parameters are as presented below:

SOBOL' G FUNCTION

Sobol' G function or simply G function [22] is one of the standard test functions used in many studies *(e.g.,* [16,23,24]). It is a strongly non-linear and non-monotonic function (JCR EC, 2010).

Sets of function coefficients, important parameter, in the descending order of ranks, for the G function configurations in this study are as follow:

a = {0.03, 0.05, 0.78, 0.79, 1, 1.25, 2.6, 2.8, 6, 40, 41, 49, 50, 52, 89, 90, 91, 92, 93, 94},

$T_{ST} = \{X_1, X_2, X_3, X_4, X_5, X_6, X_7\}$,

$\#T = 7$

Analytical expressions to calculate total effect sensitivity indices for this function can be found in [25].

MODIFIED G OR G* FUNCTION

The G function was modified by [25] to add complexity and flexibility (curvature, shift, etc.) to the function. The G* function has been used consistently in recently published works (*e.g.,* [17]).

Sets of function coefficients, important parameter, in the descending order of ranks, for the G* function configurations in this study are as follows:

a = {100, 0, 100, 100, 100, 100, 1, 0, 100, 100, 0, 100, 100, 100, 1, 100, 100, 0, 100, 1},

α = {1, 4, 1, 1, 1, 1, 0.5, 3, 1, 1, 2, 1, 1, 1, 0.5, 1, 1, 1.5, 1, 0.5},

$T_{ST} = \{X_2, X_8, X_{11}, X_{18}\}$,

$\#T = 4$

Analytical expressions to calculate total effect sensitivity indices for this function can be found in [25].

B FUNCTION

The B function is a non-additive test model developed by [1]. It has been used as a test case in a number of recent studies.

Sets of function coefficients, important parameter, in the descending order of ranks, for the B function configurations in this study

μ ={2, 2, 3, 1.5, 3, 3, 2, 2, 2, 1, 1, 2, 2, 2, 3, 3, 1.5, 3, 2, 2},

σ ={0.5, 0.5, 1, 1, 2, 2, 1, 0.5, 1.5, 2, 2, 2, 1, 1, 1, 3, 3, 3, 5, 5},

$T_{ST} = \{X_{10}, X_{20}, X_6, X_9, X_{19}, X_5, X_{16}\}$,

$\#T = 7$

Analytical expressions to calculate total effect sensitivity indices for this function can be found in [25].

M FUNCTION

The 20-parameter polynomial test function proposed by [6] has been the most regularly used test case in parameter screening experiments. The first and total effects sensitivity indices were calculated in an independent experiment using Sobol' method and verified with values published in [17] based on which following parameters were identified as important

$T_{ST} = \{X_1, X_4, X_2, X_9, X_{10}, X_8, X_5, X_3, X_6, X_7\}$,

$\#T = 10$

O FUNCTION

The O function is a 15-parameter test model proposed by [31].

Model coefficient values can be downloaded from http://www.jeremy-oakley.staff.shef.ac.uk/psa_example.txt.

Sets of important parameters were identified from the analytical sensitivity indices in [1].

$T_{ST} = \{X_{15}, X_{11}, X_{12}, X_{13}, X_{14}, X_9, X_8\}$,

$\#T$=7

TABLE 1. Summary of Sampling Strategies for the Method of Elementary Effects (EE).

Method	Trajectory Based[1]	Fix Step	Random	Principle	Authors
Morris	Y	Y	Y	--	[6] Morris (1991)
Optimized Trajectories (OT)	Y	Y	Y	Sample Spread	[16] Campolongo *et al.* (2007)
LH-OAT	Y	N	Y	LHS	[26] van Griensven *et al.* (2006)
Simplex Based	Y	N	Y	Simplex Formation	[27] Pujol (2009)
Cell Based	N	Y	Y	--	[28] Saltelli *et al.* (2009)
Radial Sampling	N	N	N	Extended OAT	[17] Campolongo et al. (2011)
Modified OT	Y	Y	Y	Sample Spread	[29] Ruano *et al.* (2012)
Constellation Based	Y	N	Y	Constellation Formation	[30] Santiago *et al.* (2012)
Quasi-OT	Y	Y	Y	Sample Spread	[15] Ge *et al.* (2015)
SU	Y	Y	Y	Uniformity and Sample Spread	[14] Khare *et al.* (2015)
Radial Morris	N	Y	Y	Radial	[20] Xiao *et al.* (2016)
Radial Quasi-Random	N	Y	Y	Radial	[20] Xiao *et al.* (2016)

1 – Trajectory based implies winding staircase type structure

TABLE 2. Average fraction of parameters passing the Chi-square goodness of fit test for a discrete uniform distribution at 5% significance level considering all sample points, for Sampling for Uniformity (SU) and enhances Sampling for Uniformity (eSU). Q = 300 was used and the averages are from 100 experiments.

	SU				eSU			
k	r = 6	r = 8	r = 10	r = 12	r = 6	r = 8	r = 10	r = 12
10	0.693	0.754	0.706	0.727	1.000	1.000	1.000	1.000
15	0.539	0.550	0.548	0.559	0.867	1.000	1.000	1.000
20	0.456	0.445	0.444	0.450	0.800	1.000	1.000	1.000
25	0.376	0.362	0.357	0.384	0.680	1.000	0.920	1.000
30	0.291	0.314	0.316	0.324	0.667	1.000	0.800	1.000

TABLE 3. Average fraction of parameters with a perfect discrete uniform distribution considering all sample points, for Sampling for Uniformity (SU) and enhances Sampling for Uniformity (eSU). Q = 300 was used and the averages are from 100 experiments.

	SU				eSU			
k	r = 6	r = 8	r = 10	r = 12	r = 6	r = 8	r = 10	r = 12
10	0.000	0.009	0.000	0.000	0.000	1.000	0.000	1.000
15	0.004	0.001	0.000	0.003	0.067	1.000	0.067	1.000
20	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000
25	0.000	0.001	0.000	0.001	0.040	1.000	0.040	1.000
30	0.000	0.000	0.000	0.000	0.000	1.000	0.000	1.000

TABLE 4. Summary of ratio of sample time generation for eSU and SU under various combinations of oversampling size (Q), number of trajectories (r) and model dimensionality (k)

Q	1	10	30	50	100	300	500	1000
r				**k = 10**				
4	0.85	0.79	0.81	0.80	0.81	0.80	0.80	0.80
8	0.83	0.83	0.83	0.82	0.83	0.82	0.81	0.84
20	0.92	0.90	0.90	0.89	0.90	0.90	0.90	0.91
40	0.97	0.93	0.94	0.93	0.94	0.94	0.93	0.92
r				**k = 15**				
4	0.75	0.81	0.78	0.78	0.76	0.79	0.80	0.77
8	0.78	0.80	0.80	0.80	0.80	0.80	0.81	0.81
20	0.90	0.88	0.89	0.88	0.88	0.89	0.90	0.88
40	0.92	0.93	0.93	0.91	0.94	0.94	0.94	0.94
r				**k = 20**				
4	0.75	0.76	0.77	0.75	0.77	0.76	0.78	0.77
8	0.73	0.74	0.75	0.75	0.75	0.76	0.75	0.76
20	0.85	0.84	0.85	0.86	0.84	0.84	0.86	0.86
40	0.96	0.93	0.92	0.93	0.92	0.92	0.93	0.91

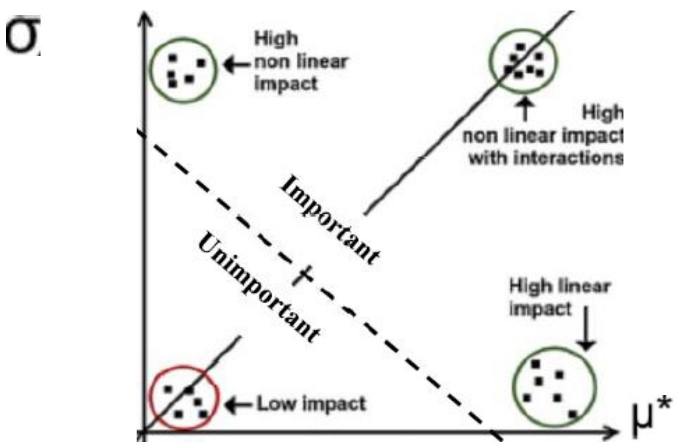

FIGURE 1. SCHEMATIC OF PARAMETER SCREENING USING METHOD OF EE (MODIFIED FROM [32])

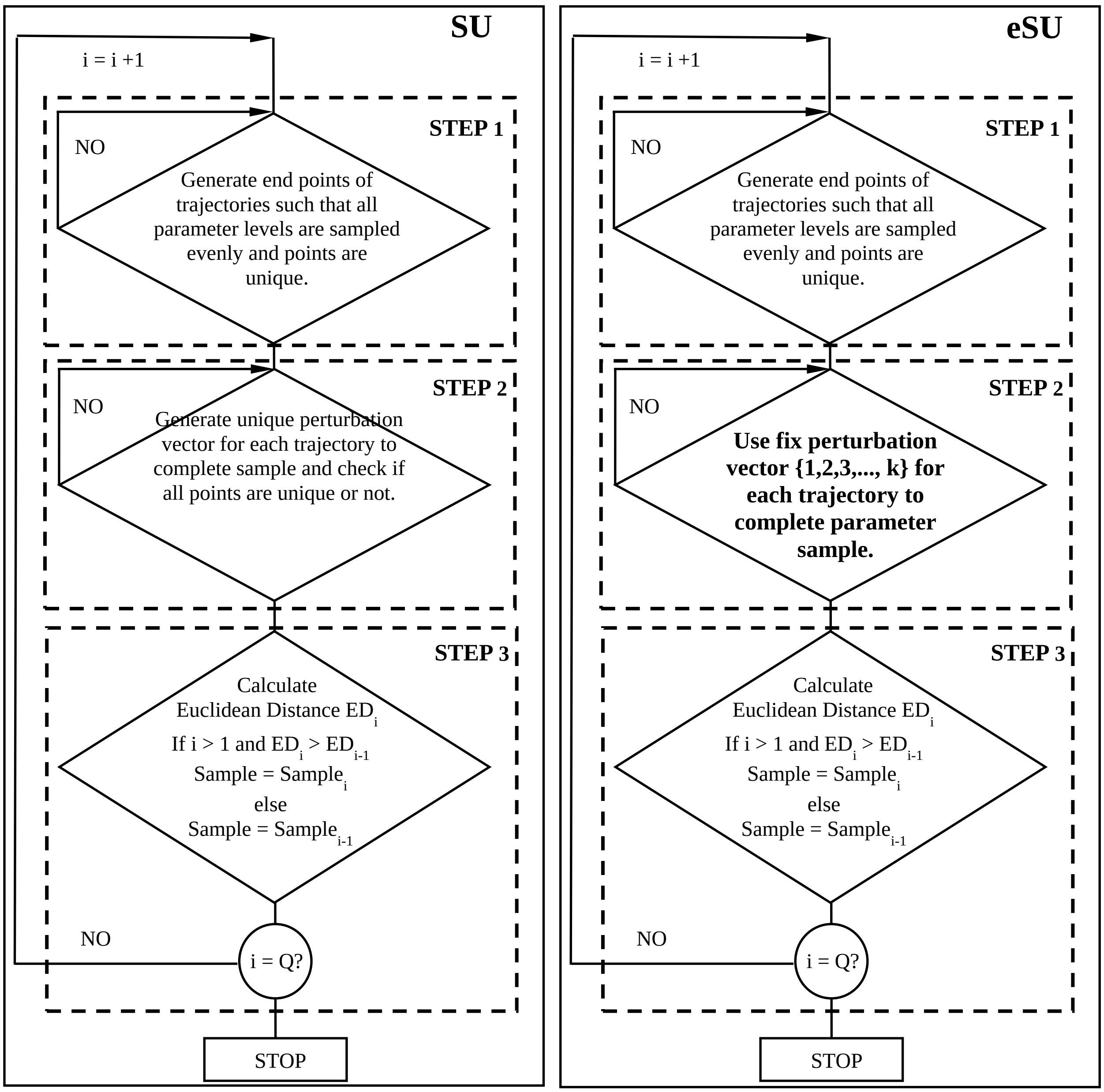

FIGURE 2. **SCHEMATIC REPRESENTATION OF ALGORITHMS USED TO GENERATE PARAMETER SAMPLES USING SU AND ESU.**

Trajectory 1

$$\begin{bmatrix} 1.00 & 0.00 & 0.33 & 1.00 \\ 0.33 & 0.00 & 0.33 & 1.00 \\ 0.33 & 0.67 & 0.33 & 1.00 \\ 0.33 & 0.67 & 1.00 & 1.00 \\ 0.33 & 0.67 & 1.00 & 0.33 \end{bmatrix} \left\{ \begin{matrix} 1 \\ 2 \\ 3 \end{matrix} \right\} \text{Perturbation Vector}$$

Trajectory 2

$$\begin{bmatrix} 0.67 & 0.33 & 0.00 & 0.00 \\ 0.00 & 0.33 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.67 & 0.00 \\ 0.00 & 1.00 & 0.67 & 0.67 \end{bmatrix} \left\{ \begin{matrix} 1 \\ 2 \\ 3 \end{matrix} \right\} \text{Perturbation Vector}$$

-

-

Trajectory r

FIGURE 3. EXAMPLE OF TRAJECTORY FORMATION USING FIXED PERTURBATION VECTOR IN ESU FOR A 4-PARAMETER MODEL.

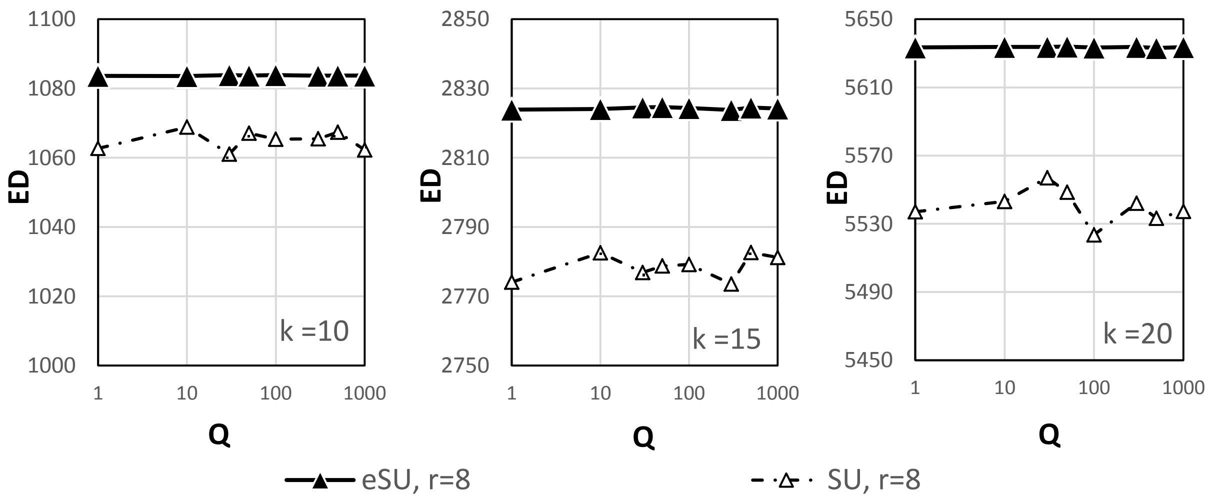

FIGURE 4. **VARIATION OF EUCLIDEAN DISTANCE (ED) OF GENERATED SAMPLE WITH OVERSAMPLING SIZE (Q) FOR THREE MODEL DIMENSIONALITIES (K) AND 8 TRAJECTORIES (*I.E.*, R = 8).**

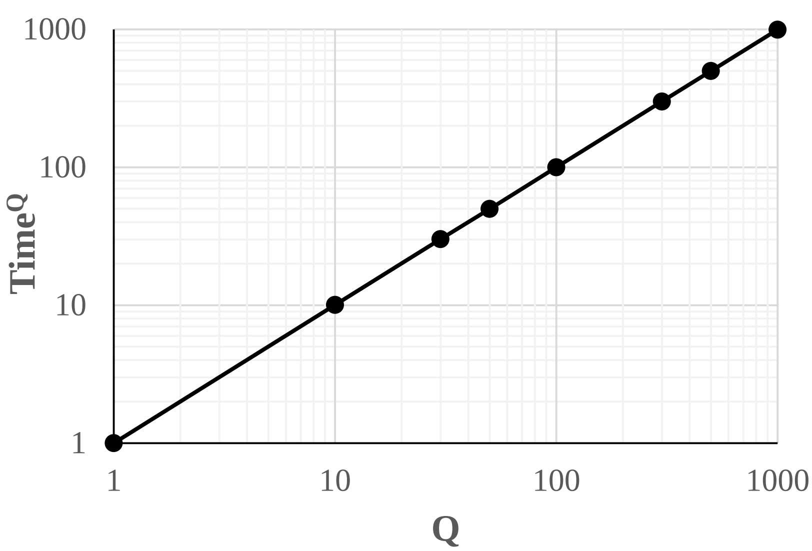

FIGURE 5. **VARIATION OF NORMALIZED SAMPLE GENERATION TIME (TIME^Q) WITH OVERSAMPLING SIZE (Q) FOR DIMENSIONALITY (K) = 15 AND NUMBER OF TRAJECTORIES (R) = 8. FOR ALL OTHER K-R COMBINATIONS TIME^Q *VS.* Q, PLOTS WERE IDENTICAL.**

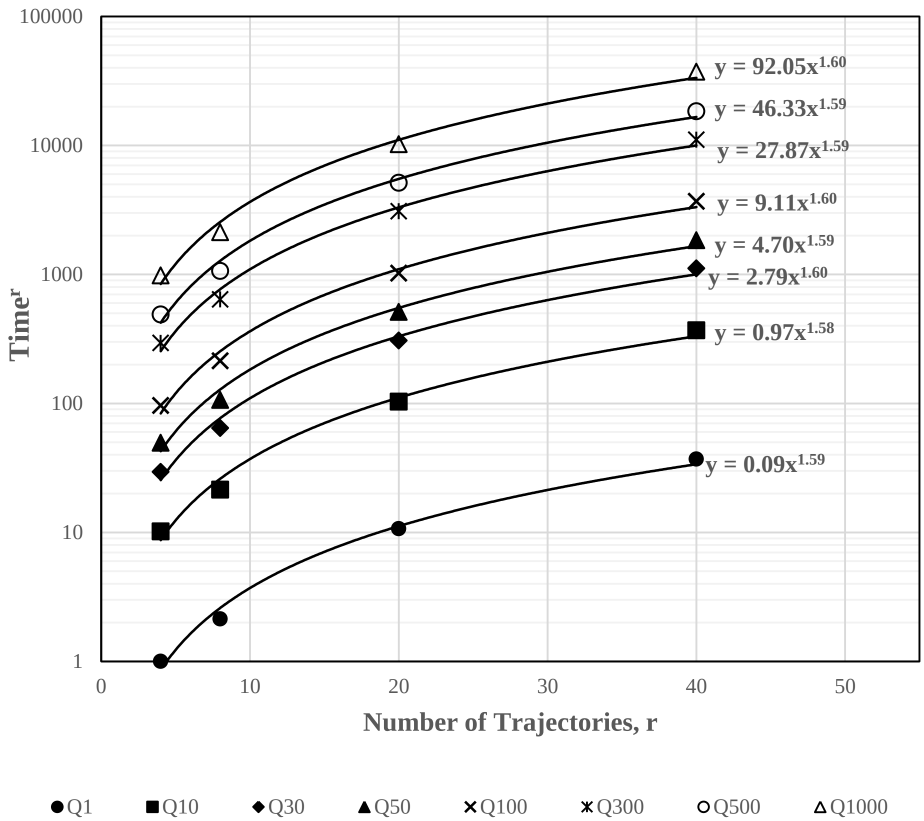

FIGURE 6. VARIATION OF NORMALIZED SAMPLE GENERATION TIME (TIME^R) WITH NUMBER OF TRAJECTORIES (R) FOR K = 15. NOTE THAT RESULTS FOR K = 10 AND K = 20 WERE SIMILAR.

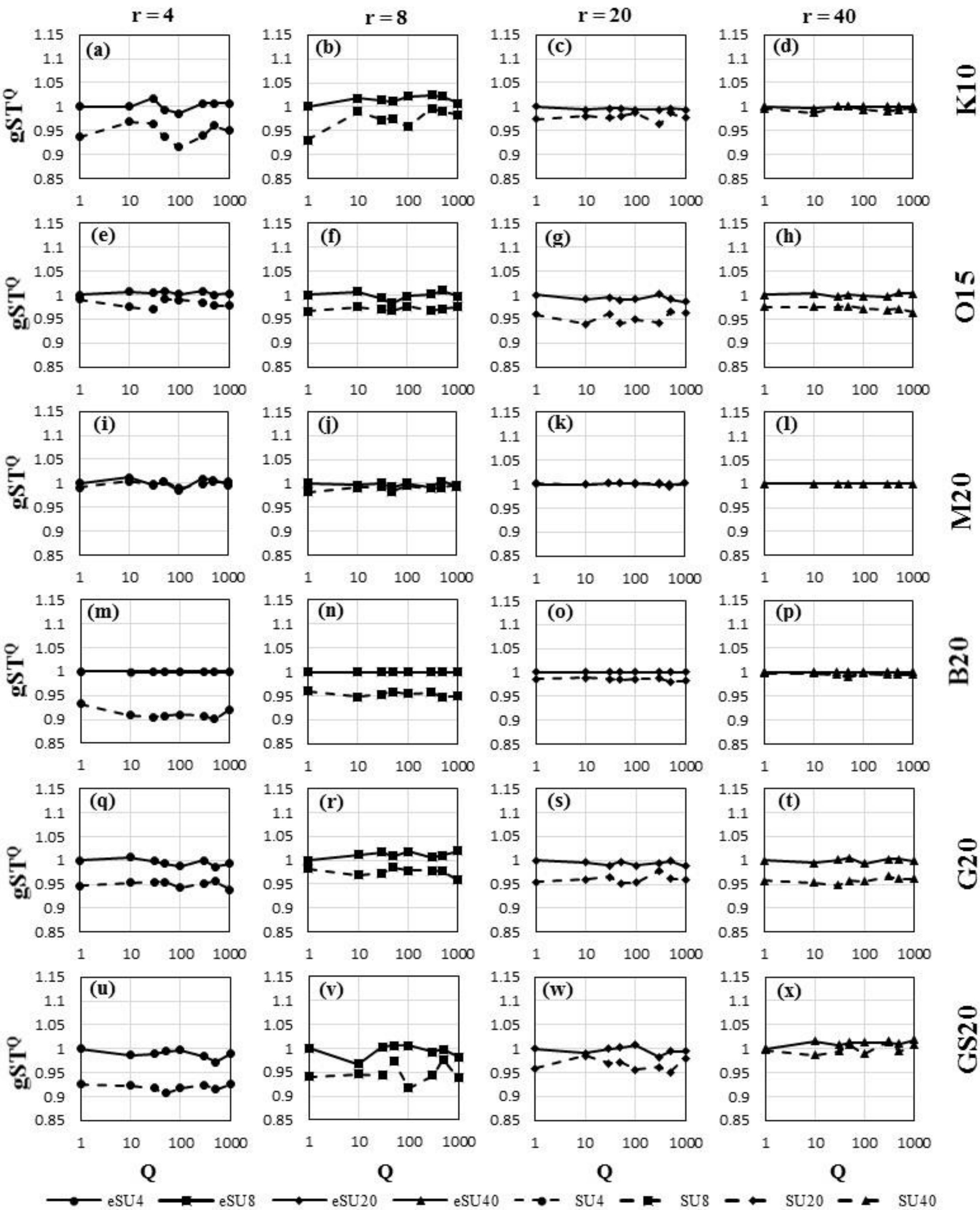

FIGURE 7. VARIATION OF NORMALIZED SCREENING EFFICIENCY GST^Q WITH Q FOR THE SIX TEST FUNCTIONS (K10, O15, M20, B20, G20, GS20) FOR TWO SAMPLING STRATEGIES (SU AND ESU) AT FOUR SAMPLE SIZES I.E. NUMBER OF TRAJECTORIES (R).

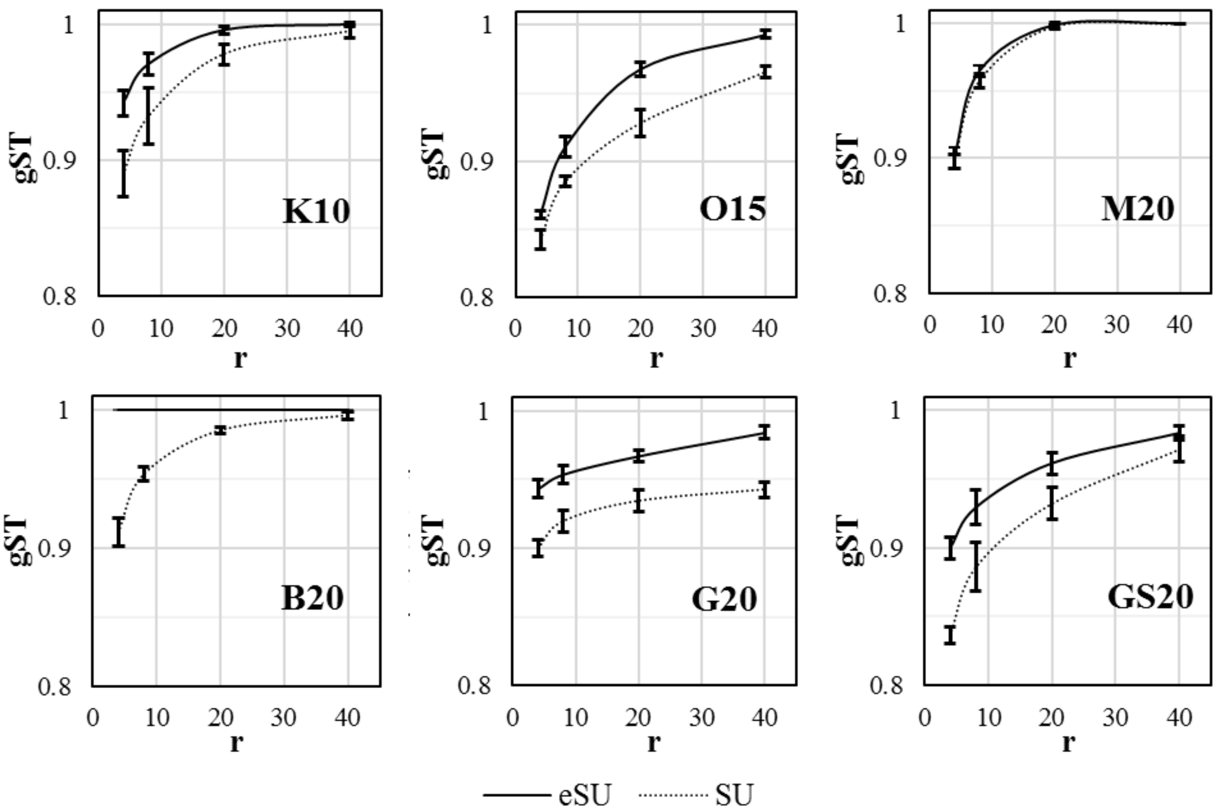

FIGURE 8. **VARIATION OF SKILL SCORE (GST) W.R.T. NUMBER OF TRAJECTORIES (R) FOR ALL SIX TEST FUNCTIONS. THE GST SCORES PLOTTED HERE WERE AVERAGED OVER ALL OVERSAMPLING SIZES (Q). ERROR BARS CORRESPOND TO STANDARD DEVIATION.**