# n Efficient Sampling-Based Method for Sensitivity and Uncertainty Analysis Through RAVEN

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## INTRODUCTION

Sensitivity analysis (SA) and uncertainty quantification (UQ) are now widely recognized as essential parts of analyses for complex nuclear systems. Plenty of well-established methodologies are already available for performing SA & UQ, such as Monte Carlo analysis, adjoint-based method, and variance decomposition [1-3].

The focus of this summary is on developing an efficient sampling-based approach to perform SA & UQ through RAVEN. RAVEN (**R**isk **A**nalysis and **V**irtual control **EN**vironment) is a software framework able to perform SA & UQ, currently under development at the Idaho National Laboratory [4]. In literature, a number of approaches have been developed to accelerate the process of SA & UQ for large complex systems, such as principal component analysis (PCA) of input space, input-output correlation analysis, and intersection subspace methods [5, 6]. The fundamental idea is to identify the dominant active directions in the parameter space prior to conducting SA & UQ. The premise is that the number of active directions is much less than the dimensionality of input space. In this work, the PCA or Karhunen-Loève expansion or SVD method is implemented in RAVEN to identify the active directions. This approach is also combined with the forward sampling approaches, such as Monte Carlo, Grid, Latin Hypercube, and Response Surface Design sampling approaches that are currently available in RAVEN, to perform SA & UQ more efficiently.

The summary is organized as follows. In following section, we present the PCA-based forward sampling approach. The effectiveness and efficiency are discussed in numerical results section. The paper then ends with a concluding summary.

## DESCRIPTION OF THE ACTUAL WORK

### Correlations of Input Parameters

In this work, PCA is employed to control the correlations of sample generation. The input parameters, represented hereinafter by $\boldsymbol{x} \in \boldsymbol{R}^n$, are assumed to have a multivariate normal distribution with mean $\boldsymbol{\mu}$ and covariance matrix $\mathbf{C} \in \boldsymbol{R}^{n\times n}$, where $n$ is the number of input parameters. In order to employ the sampling-based approach to perform SA & UQ, we need to transform the set of correlated input variables to a set of uncorrelated standard Gaussian variables $\boldsymbol{\xi}(\theta) = [\xi_1(\theta), \xi_2(\theta), \cdots, \xi_n(\theta)]$, denoted hereinafter as pseudo parameters, via the following equation:

$$\boldsymbol{x} = \boldsymbol{\mu} + \mathbf{L}\boldsymbol{\xi} \qquad (1)$$

where $\mathbf{L}$ is a lower-triangular matrix obtained via the Cholesky decomposition of $\mathbf{C} = \mathbf{L}\mathbf{L}^{\mathbf{T}}$. We can also employ PCA or singular value decomposition (SVD) in linear algebra to perform this transformation,

$$\mathbf{C} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{U}^{\mathbf{T}} \qquad (2)$$
$$\boldsymbol{x} = \boldsymbol{\mu} + \mathbf{U}\sqrt{\boldsymbol{\Sigma}}\boldsymbol{\xi} \qquad (3)$$

where $\mathbf{U}$ is $n$ by $n$ real unitary matrix and $\boldsymbol{\Sigma}$ is $n$ by $n$ diagonal matrix with non-negative real numbers. The diagonal entries $\boldsymbol{\Sigma}_{\boldsymbol{i},\boldsymbol{i}}$ of $\boldsymbol{\Sigma}$ are known as the singular values of $\mathbf{C}$.

As shown in Eq. (1) or (3), the correlations between input parameters are imposed with the matrix $\mathbf{L}$ or $\mathbf{U}\sqrt{\boldsymbol{\Sigma}}$. In Fig. 1, we have provided some illustrative results.

In some situations, the matrix $\mathbf{C}$ happens to be ill-conditioned, such as the covariance matrix for nuclear cross sections. In this case, some principal components associated with zero or small singular values, usually several orders of magnitude smaller than the largest singular values, can be neglected, while the rest of the principal components, denoted hereinafter as the active directions, can be used to perform SA & UQ more efficiently.

### PCA-Based Forward Sampling Approach

As mentioned, we have implemented the PCA approach in RAVEN, and RAVEN is now able to perform SA & UQ with the pseudo parameters in the active directions. The main procedures can be illustrated as follows:

1. Define the multivariate normal distribution $\mathcal{N}(\boldsymbol{\mu}, \mathbf{C})$ that characterizes the uncertainty in the input parameters $\{x_i\}_{i=1}^n$ or $\boldsymbol{x}$;
2. Identify the active directions via truncated SVD of input covariance $\mathbf{C}$, i.e. $\mathbf{C} = \mathbf{U_t}\boldsymbol{\Sigma_t}\mathbf{U_t^T}$, with $\mathbf{U_t} \in \boldsymbol{R}^{\boldsymbol{n}\times\boldsymbol{r}}$ and $\boldsymbol{\Sigma_t} \in \boldsymbol{R}^{\boldsymbol{r}\times\boldsymbol{r}}$;
3. Define the pseudo parameters $\{\xi_i\}_{i=1}^r$ or $\boldsymbol{\xi}$ with standard normal distributions $\mathcal{N}_1(0,1), \cdots, \mathcal{N}_r(0,1)$;
4. Draw a sample $\{\boldsymbol{\xi}_i\}_{i=1}^N$ from the distributions defined in step 3. Several methods available in RAVEN can be used

here, such as random sampling, Latin hypercube sampling and sparse grid collocation sampling;

5. Generate a sample of input parameters $\{\boldsymbol{x}_i\}_{i=1}^{N}$ via the mapping: $\boldsymbol{x}_i = \boldsymbol{\mu} + \mathbf{U_t}\sqrt{\boldsymbol{\Sigma_t}}\boldsymbol{\xi}_i, i = 1, \cdots, N$;

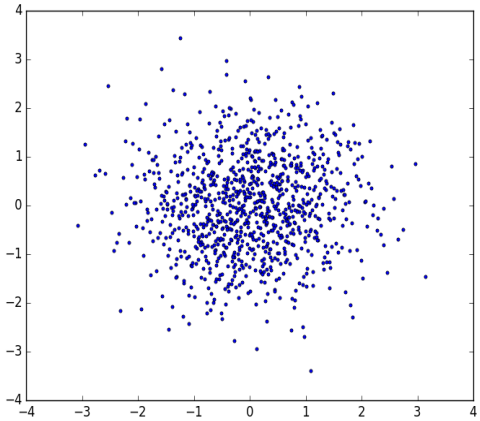
6. Propagate the sample through the computational code to produce responses of interest $\{\boldsymbol{y}_i = \boldsymbol{y}(\boldsymbol{x}_i)\}_{i=1}^{N}$;

7. Construct a reduced order model (ROM) via methods such as response surface, generalized polynomial chaos, and high-dimensional model reduction (HDMR);

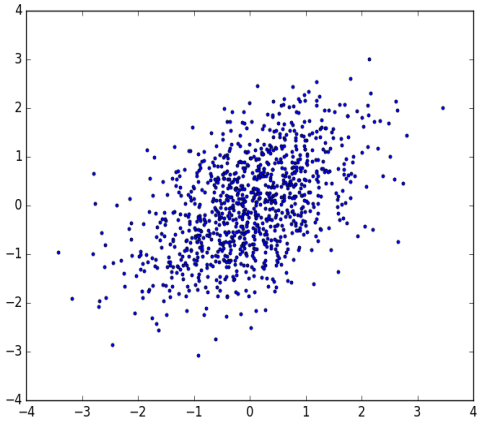
8. Perform the UQ in the responses of interest;

9. Perform the sensitivity analysis in the responses of interest with respect to the pseudo parameters via regression method, i.e. $\mathbf{S} = \frac{\boldsymbol{dy}}{\boldsymbol{dx}}$;

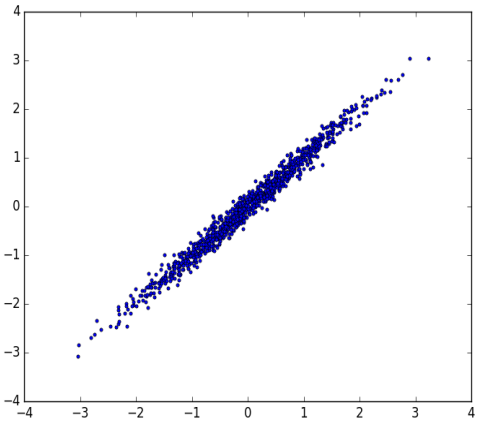
10. Compute the sensitivities of responses of interest with respect to input parameters: $\left(\mathbf{U_t}\sqrt{\boldsymbol{\Sigma_t}}\right)\mathbf{S}$.



0.0 Correlation between two standard normal distributions



0.5 Correlation between two standard normal distributions



0.99 Correlation between two standard normal distributions

Fig. 1. Examples of correlations of 0.0, 0.5, and 0.99 imposed with the proposed technique for an LHS of size $N = 1000$.

## NUMERICAL RESULTS

In this section, we present the results of the application of the proposed approach to IAEA-2D PWR benchmark [7]. The numerical solution of this benchmark is computed via RATTES$_N$AKE [8]. Several methods inside RAVEN are used to perform SA & UQ, such as Monte Carlo and HDMR. For this study, we have introduced 5% relative uncertainties, i.e. $\sigma/E = 5\%$, in capture, scattering, fission cross-sections, and neutron multiplication factor $\nu$. In addition, we have introduced 10% correlation between the energy group cross sections for each type of perturbed cross section in each material.

In Fig. 2, we present the contributions of variance in k-eigenvalue due to the size of the active directions for both HDMR and Monte Carlo methods. As observed, only few of the active directions together have the majority of contributions to the total variance. In addition, Fig. 3 and Fig. 4 illustrate the sensitivity coefficients of k-eigenvalue with respect to the pseudo parameters computed via regression method and HDMR (Sobol' indices) method. This information can then be used to re-construct the real sensitivity coefficients via step 10 in previous section. If other methods, such as response surface and sparse grid collocation with generalized polynomials chaos method, are employed, RAVEN can construct the ROM as mentioned in the step 7 in previous section. In this case, the ROM can be used to perform SA & UQ much more efficiently compared to the executions of original complex model. Currently, we are focusing on examination of the proposed method for multi-physics coupled systems, such as fuel-neutronics coupled system.

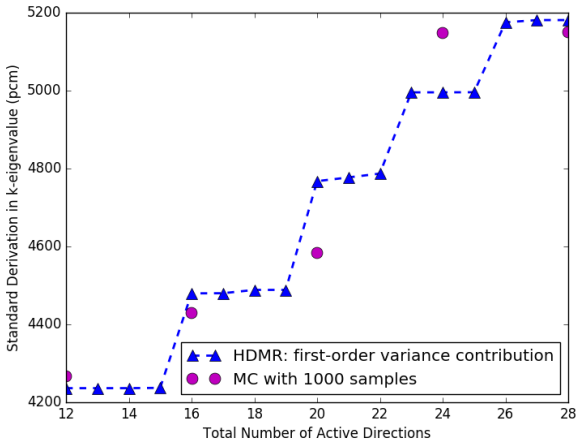



Fig. 2. Contributions of variance from the active directions

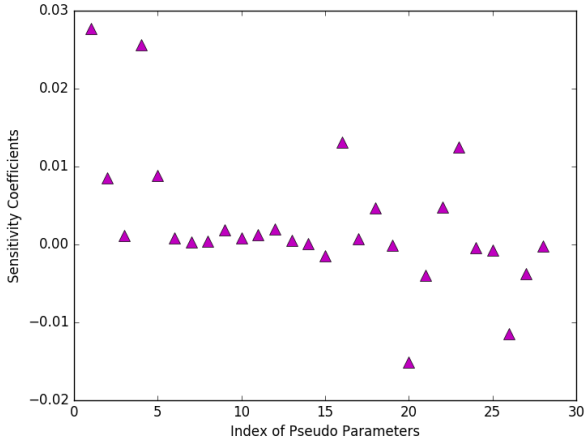



Fig. 3. Sensitivities from regression method with Monte Carlo sampling.

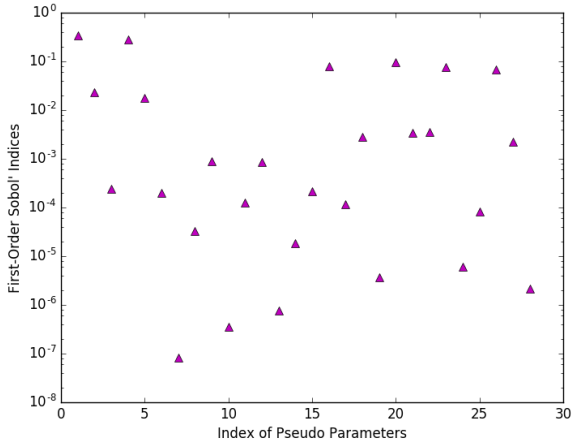



Fig. 4. First-order Sobol' indices using HDMR method.

## CONCLUSIONS

In this summary, we have presented PCA-based forward sampling approach to perform SA & UQ. The goal is to reduce the computational overhead for repetitive executions of complex nuclear systems that are generally required when performing SA & UQ. The control of correlations between input parameters is implemented in RAVEN to better represent the input relationships. In addition, we are currently examining our implementations with more realistic models, and we are also focusing on implementation some new high-dimensional input reduction techniques in RAVEN.

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