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Constrained Sensitivity Analysis for Reactor Physics Problems

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INTRODUCTION

This summary introduces an algorithm for completing sensitivity analysis that respects linear constraints placed on the associated model's input parameters. With constraints present, the degrees of freedom of input parameters are reduced, and any changes, e.g., parameter perturbations, must respect these constraints. This summary motivates the need for this algorithm, overviews the theoretical results, and offers representative numerical experiments.

The original work focuses on the sensitivity of core-wide k_{eff} [1]. In this summary, a virtual bare fast reactor whose core has three different fuel materials (U^{235}, U^{238}, Pu^{239}) is employed to demonstrate the performance of the proposed algorithm. The nominal three-group constants of fast reactors are used in the criticality analysis [2]. The objective is to calculate the sensitivity of k_∞ with respect to the volumetric ratio of fissile materials (U^{235}, U^{238}, Pu^{239}) in a multi-group format. The constraint of this analysis is that the sum of the volumetric composition ratio of the fissile materials is equal to unity.

MOTIVATION

Sensitivity analysis is widely used in many engineering applications such as model optimization, uncertainty quantification, and inference, as it allows analysts to quantify and prioritize the impact of various model parameters on model responses of interest [3]. Focusing here on the parameter perturbations aspect of any sensitivity analysis, including both forward and adjoint methods, one typically needs to perturb the parameters to quantify their individual impact on the responses of interest. This follows for both adjoint and forward methods. In a forward approach, the model parameters are perturbed and the model is re-executed and the variations in the responses of interest from their reference values are recorded, and later used to approximate the response derivatives with respect to the model parameters. In the adjoint approach, the adjoint model is first constructed, representing the mathematical dual of the forward model equations. The adjoint model is solved for a state variable, called the adjoint solution, as opposed to the forward solution. Both the adjoint and forward solutions are combined together via inner product operation to estimate the derivatives of select model response with respect to its model parameters. In this inner product formulation, one has to change one parameter at a time to estimate the derivative of the response with respect to the given parameter. Thus, essentially a forward-based approach is employed to calculate the derivatives, but applied on the inner product formulation rather than the original model. The cost of re-executing the inner product formulation is far less expensive than re-execution of the original model, which renders the adjoint-based methods superior to forward-based methods for the evaluation of first-order derivatives when the number of model parameters is very high. Thus, when constraints are enforced on the model parameter, both the forward and adjoint methods must be able to handle these constraints when perturbing the respective model parameters.

In no constraints exist, several methods are available for introducing the perturbations, such as one-at-a-time techniques often used in local sensitivity analysis, and simultaneous perturbation of all parameters using random sampling techniques as typically done in global sensitivity analysis [3]. These perturbation procedures can be implemented in a straightforward manner when the parameters are independent of each other. However, when constraints are present -- as dictated by the physics or engineering considerations -- the perturbations must satisfy these constraints. Because the number of constraints is typically much smaller in dimensionality than the number of parameters, they can be satisfied in an infinite number of ways, which could lead to non-uniqueness in the responses of interest [4-5], and ultimately to ambiguities in the downstream analyses relying on the results of this sensitivity analysis. Thus, there is a need for an algorithm that can introduce parameter perturbations for sensitivity analysis in a manner that satisfies the constraints and ensure uniqueness of the variations in the responses of interest. This is true whether one is employing forward or adjoint sensitivity analysis.

Some of the constraints that are relevant to reactor physics problems include quantities that must sum to a fixed value, e.g., isotopic percent concentrations and volume fractions in a given mixture, group-wise delayed neutron fractions, group-wise prompt neutron fractions, etc. For illustration, this summary analyzes a virtual bare reactor to estimate the sensitivity of k_∞ with respect to the fissile material volume fractions, which must sum to 1.0. The reference group-wise values are calculated using lattice physics, and the goal is to estimate the impact of their variations on k_∞.

DESCRIPTION OF PROPOSED ALGORITHM

Although the proposed algorithm has general applicability to both local and global sensitivity analysis techniques, we focus in this summary on local sensitivity methods only. For local methods, the sensitivity information is encoded in the form of a sensitivity vector, sometimes referred to as a sensitivity profile, which is equivalent to the calculus definition of a gradient, i.e., the direction of maximum ascent for the response of interest in the parameter space $\mathbb{R}^n$. If no constraints exist, the parameter perturbations can be rendered using *n* degrees of freedom, corresponding to the total number of parameters. When constraints exist however, the available number of degrees of freedom is reduced. This can be illustrated as follows for the case of linear constraints, which may be described by a set of linear equations:

$$\mathbf{A}x = b. \tag{1}$$

where $\mathbf{A} \in \mathbb{R}^{n\times m}$ is a rectangular wide matrix, such that *m* represents the number of constraints which is less than *n*. For a given model parameter perturbations Δx that satisfies the constraints, one has:

$$\mathbf{A}(x+\Delta x) = b \rightarrow \mathbf{A}\Delta x = 0 \tag{2}$$

This means that the perturbation Δx must lie in the null space of the matrix **A**. If the *m* constraints are independent, i.e., not redundant which is expected to be the case, the null space of **A** will have a dimension of *n-m*. This implies that the perturbations Δx can only vary along an *n-m* subspace. Effectively, this means that the sensitivity analysis can only assess the impact of *n-m* degrees of freedom on the response of interest. This further implies that the gradient should not have any components that are orthogonal to the null space, otherwise the constraints will be violated.

The proposed algorithm takes advantage of this observation and recasts the model input parameter perturbations in terms of these degrees of freedom via linear transformation. After completing the sensitivity analysis using standard perturbation techniques where the parameters are assumed independent, but now automatically constrained to the null space of **A**, the calculated sensitivities can be transformed back into the original parameters.

To implement this algorithm, one only needs to develop a way to generate perturbations in the null space. This can be achieved by first estimating the orthogonal complement of the null space, that is the row space of **A**. The algorithm then reduces to a simple projection exercise, where the component along the row space of **A** is removed from any proposed parameter perturbations. This procedure can be repeated *n-m* times to generate a basis for the null space, which can be used as a basis for perturbing the parameters for the sake of sensitivity analysis.

The details of the proposed algorithm may be summarized as follow:

1. Define the linear constraints as matrix **A**, then calculate $\mathbf{Q}_A$, such that $\mathbf{A}^{\mathbf{T}} = \mathbf{Q}_{\mathbf{A}}\mathbf{R}_{\mathbf{A}}$, where $\mathbf{Q}_A$ has *m* columns spanning the row space of **A**.
2. Create an orthogonal projector **P**, such that $\mathbf{P} = \mathbf{I} - \mathbf{Q}_{\mathbf{A}}\mathbf{Q}_{\mathbf{A}}^{\mathbf{T}}$.
3. Generate a random matrix $\mathbf{X} \in \mathbb{R}^{n\times(n-m)}$, and project the random matrix onto the active subspace by $\mathbf{PX}$.
4. Perform QR decomposition such that: $\mathbf{QR} = \mathbf{PX}$.
5. Let $\mathbf{Q} = [q_1 \quad q_2 \quad \ldots \quad q_{n-m}]$. Each column refers to one of the *n-m* effective degrees of freedom that are to be explored by the SA.
6. Find the acceptable step size Δ_{q_i}, which guarantees the linearity at the given local point.
7. Calculate the directional derivative along q_i with step size Δ_{q_i}.
8. Calculate the constrained gradient, $g_c = dk \times \mathbf{Q}^T$.

NUMERICAL EXPERIMENT

The focus of the numerical experiment is performing sensitivity analysis for the multiplication factor, k_∞, of a virtual fast reactor model. The model reactor is a bare reactor, whose fuel consists of three fissile materials (U^{235}, U^{238}, Pu^{239}). Its volumetric ratio sums up to unity. The three-group neutron balance equation without leakage and external sources is given by:

$$\begin{bmatrix} \Sigma_{t1}-\Sigma_{11} & -\Sigma_{21} & -\Sigma_{31} \\ -\Sigma_{12} & \Sigma_{t2}-\Sigma_{22} & -\Sigma_{32} \\ -\Sigma_{13} & -\Sigma_{23} & \Sigma_{t3}-\Sigma_{33} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \frac{1}{k_\infty} \begin{bmatrix} \chi_1\nu\Sigma_{f1} & \chi_1\nu\Sigma_{f2} & \chi_1\nu\Sigma_{f3} \\ \chi_2\nu\Sigma_{f1} & \chi_2\nu\Sigma_{f2} & \chi_2\nu\Sigma_{f3} \\ \chi_3\nu\Sigma_{f1} & \chi_3\nu\Sigma_{f2} & \chi_3\nu\Sigma_{f3} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}$$

Ignoring upscattering, $\Sigma_{21}, \Sigma_{31}, \Sigma_{32}$ and thermal neutron spectrum, χ_3, the eigenvalue, k_∞, is calculated by finding the value which makes the determinant of the homogeneous equation zero.

$$k_\infty = \frac{(\chi_1\Sigma_{12} + \chi_2\Sigma_{R1})(\nu\Sigma_{f3}\Sigma_{23} + \nu\Sigma_{f2}\Sigma_{R3}) + \chi_1\Sigma_{R2}(\nu\Sigma_{f3}\Sigma_{13} + \nu\Sigma_{f1}\Sigma_{R3})}{\Sigma_{R1}\Sigma_{R2}\Sigma_{R3}}$$

where, $\Sigma_{Ri} = \Sigma_{ti} - \Sigma_{ii}(i = 1,2,3)$ is a removal cross-section.

The three-group constants are obtained by averaging techniques based on multigroup calculations [2]. The volumetric composition of the core is 30% fuel, 50% coolant (Na), and 20% structural material (Fe). These fractions of the fissile materials are given by a vector: $VF = [VF_{49} \quad VF_{25} \quad VF_{28}]^T$, where 49, 25, 28 are corresponding fissile materials Pu^{239}, U^{235}, and U^{238}

respectively. The constraint is: $\sum_i VF_i = 1, (i = 49, 25, 28)$, or in matrix format:

$$[1 \quad 1 \quad 1]VF = 1.0$$

The model employed in this analysis use the following values for the volumetric fractions of the fuel isotopes:

$$VF = [0.50 \quad 0.30 \quad 0.20]$$

The optimum step size must be determined, because too small of a step size may cause numerical errors and too big may not capture local variations. This can be obtained by analyzing variations in a step size:

$$\frac{\partial k_\infty}{\partial q_i} = \frac{f(x + \varepsilon q_i) - f(x)}{\varepsilon}$$

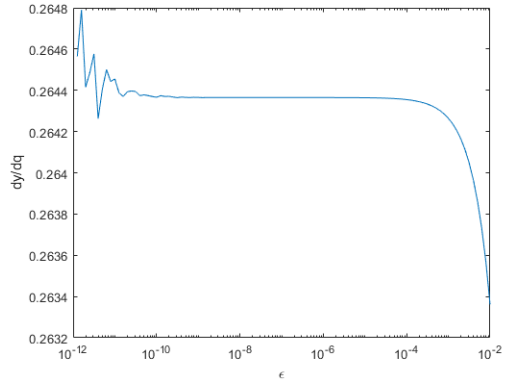

Fig. 1. Derivative plot with different ε values

Fig.1 shows a representative result for this analysis for the q_1 direction. The result indicates that $10^{-8} < \varepsilon < 10^{-4}$ is an acceptable size for a sensitivity analysis using absolute perturbations. In the same way, relative perturbations indicate that $10^{-10} < \varepsilon < 10^{-6}$ is an acceptable step size. For the sake of brevity, this analysis focuses on absolute perturbations only.

The degree of freedom in this analysis is 2, since the whole space has three dimensions and one constraint is present. The proposed algorithm is demonstrated by the following steps.

The normalized constraint is given by (after normalization to have unit norm):

$$\mathbf{Q}_A = [0.5774 \quad 0.5774 \quad 0.5774] \rightarrow \| \mathbf{Q}_A \| = 1.0$$

To respect the constraint, a random sample, **X** must be projected onto the null space of the constraint. The projection matrix is given by:

$$\mathbf{P} = (\mathbf{I} - \mathbf{Q}_A{}^T \mathbf{Q}_A) = \begin{bmatrix} 0.6667 & -0.3333 & -0.3333 \\ -0.3333 & 0.6667 & -0.3333 \\ -0.3333 & -0.3333 & 0.6667 \end{bmatrix}$$

The random sample and the projected sample are given by:

$$\mathbf{X} = \begin{bmatrix} 1.7293 & 1.0671 \\ 0.0671 & -0.9584 \\ -0.9238 & 1.5342 \end{bmatrix}$$

$$\mathbf{PX} = \begin{bmatrix} 1.4384 & 0.5195 \\ -0.2238 & -1.5061 \\ -1.2147 & 0.9866 \end{bmatrix}$$

A QR decomposition yields two orthogonal directions which are orthogonal to the constraint:

$$\mathbf{Q} = \begin{bmatrix} -0.7587 & 0.3017 \\ 0.1180 & -0.8079 \\ 0.6407 & 0.5062 \end{bmatrix}$$

The resulting derivatives of k_∞ along each of the two directions are given by:

$$\frac{\partial k}{\partial q} = [-0.5046 \quad 0.1538]$$

RESULTS

A representative result for the three-group fast reactor model using absolute perturbations is given by:

$$g_c = [0.4292 \quad -0.1838 \quad -0.2454]$$

As explained earlier, the goal is to create perturbations that ensure uniqueness of the response variations. Hence, to verify the implementation, the algorithm is repeated several times with different randomly generated parameter perturbations, as contained in the matrix **X**. The calculated gradient for a representative set of random perturbations are given here:

$$g_{c1} = [0.4292 \quad -0.1838 \quad -0.2454]$$
$$g_{c2} = [0.4292 \quad -0.1838 \quad -0.2454]$$
$$g_{c3} = [0.4292 \quad -0.1838 \quad -0.2454]$$
$$g_{c4} = [0.4292 \quad -0.1838 \quad -0.2454]$$

By definition, the gradient is expected to coincide with the direction that results in the maximum change. For the next test, many random candidate perturbations are created

and forced to satisfy the constraints. The angle between the perturbations and the gradient is calculated.

Fig. 2 shows the change in k_∞ against the angle between the perturbations and the gradient. The orange line presents a cosine function as a reference. As expected, the direction of the gradient makes the maximum change in the response of interest. The larger angle between the perturbations and the gradient causes the smaller change in k_∞.

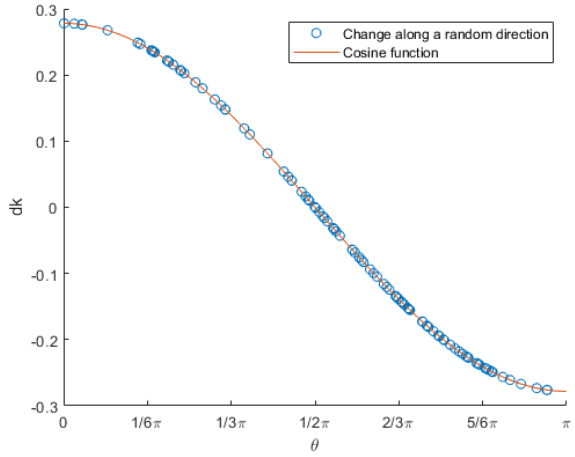

Fig. 2. k_∞ variations along randomized parameter directions vs. angle between calculated gradient and the randomized parameter directions

CONCLUSION

This summary introduced an algorithm, which allows one to generate constrained perturbations based on linear constraints. The main idea behind this algorithm is to retain only components that satisfy the constraints. Using this algorithm one can ensure that all parameter perturbations are consistent with the existing constraints. Results show that the proposed algorithm generates unique estimate of the gradient, employed in local sensitivity analysis, and the gradient is shown to satisfy the commonly known property of being the direction of maximum change. Future work will focus on illustrating the performance of this algorithm to global sensitivity analysis, and also for downstream analyses relying on the results of sensitivity analysis, e.g., uncertainty quantification and inference.

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