A method for spatial sensitivity analysis

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1. Introduction

A proper uncertainty quantification study must characterize the importance of each of the various inputs to the physical model. This is commonly referred to as sensitivity analysis. In realistic applications with many inputs, sensitivity analysis is often performed – by using prior knowledge or heuristically perturbing a nominal input value – to reduce the number of parameters included in the uncertainty quantification to something tractable. However, such an approach is not feasible when the model input is a field, such as a spatially varying boundary condition or material property.

Mathematically, we can express the Frechet derivative of a model output with respect the field input. But this is not useful for computation; once the input field is discretized on a mesh, the Frechet derivative becomes a vector with as many components as mesh points. When model evaluations are expensive, independently perturbing the field at each mesh point is infeasible. Instead, we would like a small set of spatially varying functions that indicate where the input should be perturbed to create the largest change in the output on average.

In this work, we describe a method for determining such a set of functions. We assume the model output is a scalar quantity of interest. (This can be relaxed somewhat to a handful of scalars, but we avoid the case of a field output.) We first formally perturb the input by a Gaussian random field, which is represented and parameterized by a truncated Karhunen-Loeve expansion. We then sample the Jacobian of the quantity of interest with respect to the parameters of the perturbation. These Jacobians can be computed with adjoints or finite differences if a closed form for the Frechet derivative is not available.

From the ensemble of Jacobian evaluations, we can determine the directions in the synthetic parameter space along which the quantity of interest varies the most; the directions come from a specific eigenvalue computation related to the ensemble of Jacobians. By using the components of each direction as coefficients of a linear combination of the Karhunen-Loeve basis vectors, we construct the *spatial sensitivity vectors* (SSVs) for sensitivity analysis. The associated eigenvalues order the SSVs according to which affect the quantity of interest the most on average.

For further reading on the general subject of sensitivity analysis, see Saltelli *et al.* (2008). The methods described there seek a subset of *important* parameters from the original parameters. The method we propose for spatial sensitivity analysis is closely related to the procedure described in Constantine & Wang (2012) for dimension reduction in multivariate function approximation. This differs from subset selection methods by seeking directions in the input parameters space (i.e., linear combinations of the original parameters) that can be characterized as important. This was applied in Chen *et al.* (2011) to study geometric perturbations of an airfoil.

The remainder of the report is structured as follows. In Section 2 we set up a model problem with a spatially varying input and describe the procedure to construct the SSVs. We demonstrate the effectiveness of the procedure with a numerical example in Section 3, and we provide concluding remarks and directions for future work in Section 4.

2. Problem setup

We consider a general differential equation as a representative physical problem. To keep the notation simple, we assume no time dependence in the solution, though this is not strictly necessary. Let $\mathcal{X} \subset \mathbb{R}^2$ be a spatial domain; we seek $u = u(x)$ that satisfies

$$f(u, a) \;=\; 0, \qquad x \in \mathcal{X}, \tag{2.1}$$

with appropriate boundary conditions. The spatially varying model input $a = a(x)$ may affect the operator or forcing terms; the case of the spatially varying boundary conditions is equivalent. Define $q = q(u) \in \mathbb{R}$ to be a scalar quantity of interest computed from the solution u.

We formally perturb the inputs a by a zero-mean Gaussian random field. Note that this differs conceptually from a specific perturbation $a + \Delta a$ by introducing an abstract space that characterizes a class of perturbations. The issue that arises when using a specific perturbation is how to choose Δa; should it be a constant or spatially varying? How might it vary spatially? Should all regions be perturbed in the same direction? By choosing the perturbation to be a random field, we avoid these questions to some extent.

In particular, we choose the random field to be a finite term Karhunen-Loeve expansion. The expansion coefficients become an added set of coordinates that perturb a by the orthonormal Karhunen-Loeve modes, which are ordered by how much energy they carry in the physical domain. In effect, this is a form of dimension reduction, taking the coordinates of the perturbation from one per grid point to one per Karhunen-Loeve mode. If the number of terms in the expansion is equal to the number of grid points, then there is no reduction. However, if one can justify a correlation length in the input that is larger than the grid spacing, then it may be possible to truncate at far fewer modes than grid points. This is what we typically do in practice. However, the truncation does restrict the class of perturbations, and in principle this restriction may leave out important spatial perturbations. We use the Karhunen-Loeve expansion to explore the space of perturbations with the chosen correlation length. We will use the results of that exploration to determine the spatial sensitivity vectors.

Define

$$g \;=\; g(x, \boldsymbol{\xi}) \;=\; \sum_{i=1}^{m} \xi_i \, \phi_i(x), \qquad \boldsymbol{\xi} = [\xi_1, \ldots, \xi_m]^T. \tag{2.2}$$

The $\phi_i(x)$ are the first m eigenfunctions of the exponential covariance kernel

$$\mathcal{C}(x, y) \;=\; \exp\left(-\frac{|x_1 - y_1|}{\ell_1} - \frac{|x_2 - y_2|}{\ell_2} \right) \tag{2.3}$$

with correlation lengths ℓ_1 and ℓ_2 along respective coordinates in $\mathcal{X}$. Formally, $\boldsymbol{\xi}$ is a vector of independent standard Gaussian random variables. However, for our purposes they are merely parameters that characterize a class of admissible perturbations.

Note that the choice of the exponential covariance with exponent equal to one is important. Realizations from this field are not smooth and will more easily identify local regions in space.

We use g to model an unknown perturbation to a. In other words, we replace the model 2.1 by a perturbed model

$$f(u, a + \sigma g) \;=\; 0, \qquad x \in \mathcal{X}, \tag{2.4}$$

where σ controls magnitude of the perturbations†. We assume that the model remains well-posed over the measure of this perturbation.

Under the perturbed problem 2.4, we have the following parametric dependence in the quantity of interest q,

$$q \;=\; q(u) \;=\; q(u(g)) \;=\; q(u(g(\boldsymbol{\xi}))) \;=\; q(\boldsymbol{\xi}). \tag{2.5}$$

The sensitivity can now be studied in terms of changes in q with respect to the coefficients of the Karhunen-Loeve expansion as opposed to the mesh points. As noted above, we expect m to be much smaller than the number of mesh points. We can express sensitivities in q by the m-term Jacobian $\partial q/\partial \xi_i$. Define the vector of the Jacobian transposed as

$$\mathbf{j} \;=\; \mathbf{j}(\boldsymbol{\xi}) \;=\; \begin{bmatrix} \frac{\partial q}{\partial \xi_1} \\ \vdots \\ \frac{\partial q}{\partial \xi_m} \end{bmatrix}. \tag{2.6}$$

For the Gaussian measure $d\boldsymbol{\xi}$, define the $m \times m$ matrix of integrals,

$$\mathbf{C} \;\equiv\; \int_{\mathbb{R}^m} \mathbf{j}\,\mathbf{j}^T \, d\boldsymbol{\xi}. \tag{2.7}$$

The matrix $\mathbf{C}$ measures the average squared change in q over the class of perturbations. Note that this is not related to the Hessian. Denote the eigendecomposition of $\mathbf{C}$ by

$$\mathbf{C} \;=\; \mathbf{W}\Lambda\mathbf{W}^T, \quad \mathbf{W} = \begin{bmatrix} \mathbf{w}_1 & \cdots & \mathbf{w}_m \end{bmatrix}, \quad \Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_m). \tag{2.8}$$

Note that

$$\lambda_k \;=\; \mathbf{w}_k^T \mathbf{C} \mathbf{w}_k \;=\; \int_{\mathbb{R}^m} (\mathbf{w}_k^T \mathbf{j})\, d\boldsymbol{\xi}, \quad k = 1, \ldots, m. \tag{2.9}$$

Thus, if λ_k is relatively large, then on average we expect perturbations of g along the direction $\mathbf{w}_k$ in the space of $\boldsymbol{\xi}$ to have greater effect on the quantity of interest q.

We will use the eigenvectors $\mathbf{w}_k$ to construct the m spatial sensitivity vectors, which we denote as $\psi_k(x)$, $k = 1, \ldots, m$. In particular

$$\psi_k(x) = \sum_{i=1}^{m} \mathbf{w}_{ik}\, \phi_i(x), \tag{2.10}$$

where $\mathbf{w}_{ik}$ is the ith component of the kth eigenvector, and $\phi_i(x)$ is the ith Karhunen-Loeve basis from (2.2).

One can interpret the SSV ψ_k as the spatially varying perturbation to the input a in (2.1) that produces the kth largest change in the quantity of interest q, on average. Therefore, the first few SSVs can justifiably be used in an efficient sensitivity analysis. Also, visualizing the SSVs can provide insight into the physical problem, as will be demonstrated in Section 3.

2.1. *Implementation*

In practice, one cannot exactly compute the integrals in the matrix $\mathbf{C}$ from (2.7), and they must be approximated by numerical quadrature. We propose to use a simple Monte Carlo method since high precision is not necessary to reveal to gross features of the SSVs.

† The multiplier σ could itself be a spatially varying function representing prior knowledge of the effects of a.

Denote a set of p points from the space of parameters $\boldsymbol{\xi}$ by

$$\boldsymbol{\xi}^{(k)} \;=\; [\,\xi_1^{(k)}, \ldots, \xi_m^{(k)}\,]^T \;\in\; \mathbb{R}^m, \quad k = 1, \ldots, p, \tag{2.11}$$

and define the Jacobian evaluations $\mathbf{j}_k \;=\; \mathbf{j}(\xi^{(k)})$. Then the integrals from (2.7) can be approximated by

$$\mathbf{C} \;\approx\; \tilde{\mathbf{C}} \;=\; \frac{1}{p}\sum_{k=1}^{p} \mathbf{j}_k\,\mathbf{j}_k^T \;=\; \frac{1}{p}\,\mathbf{J}\,\mathbf{J}^T, \tag{2.12}$$

where $\mathbf{J}$ is an $m \times p$ matrix defined as

$$\mathbf{J} = \begin{bmatrix} \mathbf{j}_1 & \cdots & \mathbf{j}_p \end{bmatrix}. \tag{2.13}$$

The eigenvectors and square roots of the eigenvalues of $\tilde{\mathbf{C}}$ are revealed by a thin singular value decomposition of the matrix $p^{-1/2}\,\mathbf{J}$,

$$\frac{1}{\sqrt{p}}\mathbf{J} = \mathbf{U}\Sigma\mathbf{V}^T, \tag{2.14}$$

where $\mathbf{U} \approx \mathbf{W}$. To verify this, note that

$$\tilde{\mathbf{C}} \;=\; \frac{1}{p}\,\mathbf{J}\,\mathbf{J}^T \;=\; \left(\frac{1}{\sqrt{p}}\mathbf{J}\right)\left(\frac{1}{\sqrt{p}}\mathbf{J}^T\right) \;=\; \mathbf{U}\Sigma\mathbf{V}^T\,\mathbf{V}\Sigma\mathbf{U}^T \;=\; \mathbf{U}\Sigma^2\mathbf{U}^T, \tag{2.15}$$

which is an eigenvalue decomposition. Compare this to (2.8) to see that $\mathbf{U} \approx \mathbf{W}$ and $\Sigma^2 \approx \Lambda$. In practice, we use $\mathbf{U}$ in place of $\mathbf{W}$ when constructing the SSVs in (2.10), and we use the squares of the singular values $\mathrm{diag}\,(\Sigma)$ to determine their relative importance. Current research seeks a bound on the errors in the SSVs computed with the approximation $\tilde{\mathbf{C}}$.

In some cases, the exact derivative computation $\mathbf{j}(\boldsymbol{\xi})$ may need to be approximated. We propose to use either finite difference approximations or adjoint computations if available. In the example in the next section, we will use adjoints.

3. Example

Next we demonstrate the computation and use of the SSVs on a simple model problem. Consider the square domain $\mathcal{X} = [0,1]^2$ shown in Figure 1 with boundary segments denoted by Γ_1 and Γ_2. Let $u = u(x,a)$ solve

$$\begin{aligned} -\nabla\cdot(a\,\nabla u) &= 1, \quad (x_1,x_2) \in [0,1]^2, \\ u &= 0, \quad x \in \Gamma_1, \\ n\cdot(a\,\nabla u) &= 0, \quad x \in \Gamma_2, \end{aligned} \tag{3.1}$$

where n is the normal vector to Γ_2. The coefficients a take one value on the top half of the domain and a smaller value on the bottom half,

$$\log(a) \;=\; \begin{cases} \log(10), & x_2 > 0.5 \\ \log(0.01), & x_2 \le 0.5. \end{cases} \tag{3.2}$$

The use of logarithms will ensure that the coefficients perturbed by a Gaussian random field will remain positive. The quantity of interest we consider is

$$q \;=\; \int_{\Gamma_2} u\,dx_2. \tag{3.3}$$

By reasoning about the nature of the solution u as a function of the coefficients a, we expect that variations in the region of the domain with the smaller coefficient $\log(0.01)$

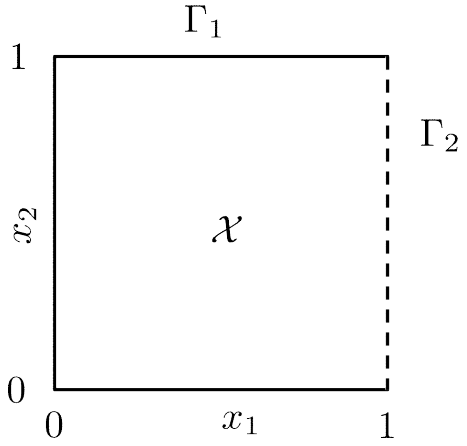


FIGURE 1. The physical domain for (3.1). The solid line corresponds to Γ_1 where the solution has homogeneous Dirichlet boundary conditions. The dashed line corresponds to Γ_2 where the solution has homogeneous Neumann boundary conditions.

to have much greater impact on the quantity of interest. This hypothesis will be verified by the SSVs.

Let g be the Gaussian process defined by (2.2) with covariance function (2.3). We take $m = 250$ terms in the expansion of g, where the correlation length parameters are $\ell_1 = 0.1$ and $\ell_2 = 0.05$. The Gaussian perturbation is formally scaled by $\sigma = 0.1$.

3.1. *Finite element discretization*

Given a value for the input parameters $\boldsymbol{\xi}$, we discretize the elliptic problem with a standard linear finite element method using MATLAB's PDE Toolbox. The discretized domain has 34320 triangles and 17361 nodes; the eigenfunctions $\phi_i = \phi_i(x)$ from (2.2) are approximated on this mesh. The matrix equation for the discrete solution $\mathbf{u} = \mathbf{u}(\boldsymbol{\xi})$ at the mesh nodes is

$$\mathbf{K}\mathbf{u} = \mathbf{f}, \tag{3.4}$$

where $\mathbf{K} = \mathbf{K}(\boldsymbol{\xi})$ is symmetric and positive definite for all $\boldsymbol{\xi}$. We can approximate the linear functional q as

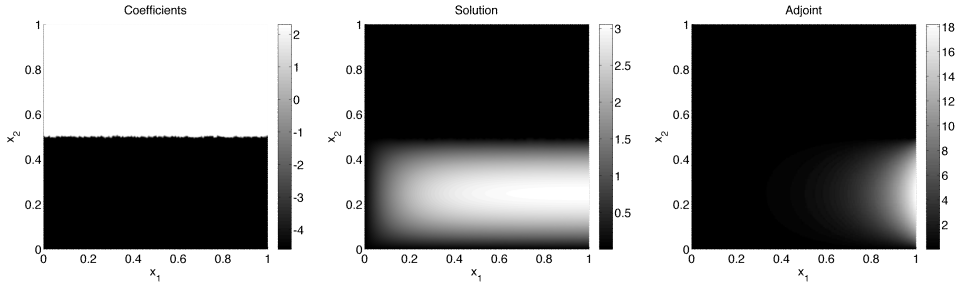
$$q \approx \mathbf{c}^T\mathbf{u}, \tag{3.5}$$

where the elements of $\mathbf{c}$ are zero except corresponding to nodes on Γ_2. The nonzero elements are constant and scaled so that they sum to one; note that $\mathbf{c}$ does not depend on $\boldsymbol{\xi}$. From now on, we will take this approximation as the definition of q.

3.2. *Adjoint variables & Jacobian*

Since the quantity of interest can be written as a linear functional of the solution, we can define adjoint variables that will help us compute the Jacobian of q with respect to the input parameters $\boldsymbol{\xi}$. Notice that we can write

$$q = \mathbf{c}^T\mathbf{u} = \mathbf{c}^T\mathbf{u} - \mathbf{y}^T(\mathbf{K}\mathbf{u} - \mathbf{f}), \tag{3.6}$$



(a) (b) (c)

FIGURE 2. 2(a) The log of the coefficients $\log(a)$. 2(b) The solution of (3.1). 2(c) The adjoint solution.

for any constant vector $\mathbf{y}$. Taking the derivative of (3.6) with respect to the input ξ_i, we get

$$\begin{aligned}\frac{\partial q}{\partial \xi_i} &= \mathbf{c}^T \left(\frac{\partial \mathbf{u}}{\partial \xi_i} \right) - \mathbf{y}^T \left(\frac{\partial \mathbf{K}}{\partial \xi_i} \mathbf{u} + \mathbf{K} \frac{\partial \mathbf{u}}{\partial \xi_i} \right) \\ &= \left(\mathbf{c}^T - \mathbf{y}^T \mathbf{K} \right) \left(\frac{\partial \mathbf{u}}{\partial \xi_i} \right) - \mathbf{y}^T \left(\frac{\partial \mathbf{K}}{\partial \xi_i} \right) \mathbf{u}\end{aligned}$$

If we choose $\mathbf{y}$ to solve the adjoint equation

$$\mathbf{K}^T \mathbf{y} = \mathbf{c}, \tag{3.7}$$

then

$$\frac{\partial q}{\partial \xi_i} = -\mathbf{y}^T \left(\frac{\partial \mathbf{K}}{\partial \xi_i} \right) \mathbf{u}. \tag{3.8}$$

To approximate the Jacobian at the point $\boldsymbol{\xi}$, we compute the finite element solution with (3.4), solve the adjoint problem (3.7), and compute the components with (3.8). The derivative of $\mathbf{K}$ with respect to ξ_i is easy compute from the derivative of $a(x, \boldsymbol{\xi})$. With these evaluations of the Jacobian, the matrix $\tilde{\mathbf{C}}$ is computed as in (2.12) with $p = 10000$ points.

3.3. *Results*

The first four Karhunen-Loeve modes are shown in Figure 3. Compare these to the first four SSVs, shown in Figure 4. One can see the localized features of the SSVs, which correspond to the spatial regions of sensitivity for the quantity of interest with respect to the spatially varying input.

In Figure 5 we plot the singular values of the Karhunen-Loeve decomposition compared to those of the matrix $\mathbf{J}$. With respect to the chosen quantity of interest, there is only a single dominant direction in the parameter space. Also, note that the singular values of $\mathbf{J}$ decay much more rapidly than the Karhunen-Loeve singular values.

As a final demonstration of the SSVs, Figure 6 plots the value of the quantity of interest q along the dominant SSV compared to random normalized directions in the space of $\boldsymbol{\xi}$. One can clearly see that changes in q along the SSV are substantially greater than in the randomly chosen directions. The parameter s on the horizontal axis scales the normalized directions.

As an aside, the quantity of interest is very nearly linear with respect to the parameter in this particular example. Additional experiments (not shown) reveal that s must be

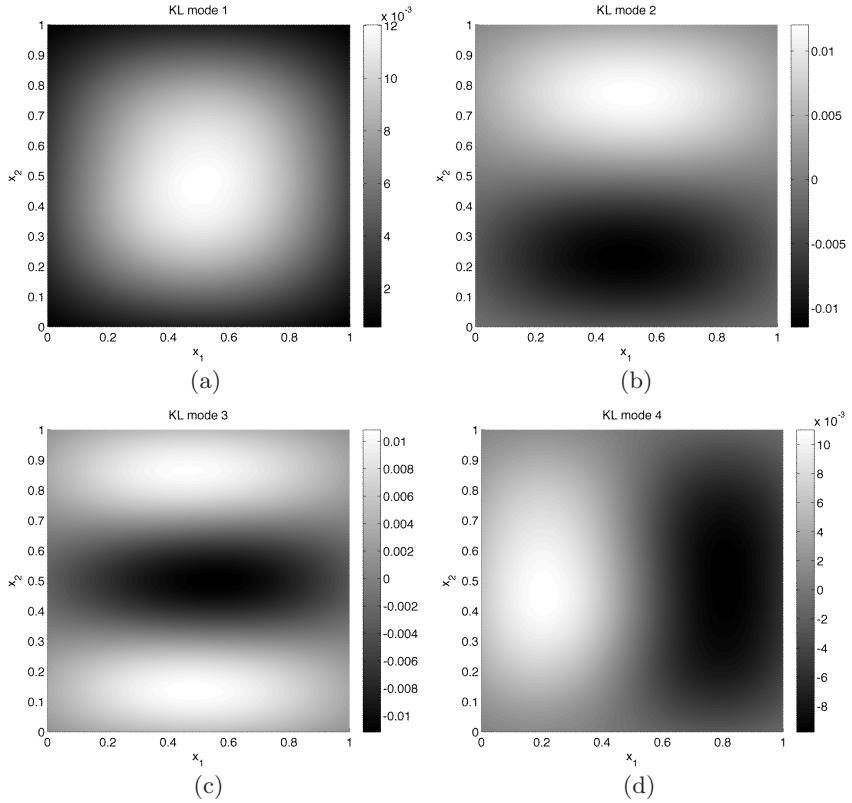


FIGURE 3. The first four Karhunen-Loeve basis functions from (2.2).

made very large (± 10) before the nonlinear effects are noticeable. The large separation between the first and second singular value of $\mathbf{J}$ in Figure 5 supports this idea. If such dominance is known a priori, then one is justified to compute only one gradient evaluation $\mathbf{j}(\boldsymbol{\xi})$ at $\boldsymbol{\xi} = 0$ and use this as the coefficients of the SSV. However, this is rarely known in practice.

4. Conclusion

We have presented a method for sensitivity analysis for a scalar quantity of interest from a model with a spatially varying input. The result is a set of vectors we call the spatial sensitivity vectors which indicate the regions in the physical domain where perturbations result in the greatest change in the quantity of interest. We have demonstrated this approach on a simple model elliptic problem with a spatially varying coefficient.

The reader may have noticed that constructing the spatial sensitivity vectors required many evaluations of the model itself. We are currently seeking to understand the minimum number of gradient evaluations necessary to get a good approximation of the SSVs sufficient for a useful sensitivity analysis. As mentioned in the example, if it is known a priori that the dependence of the quantity of interest is nearly linear with respect to the synthetic parameters of the perturbation, then this one only needs a single evaluation of the Jacobian. However, if the dependence on the synthetic parameters is strongly nonlinear, then many samples may be required.

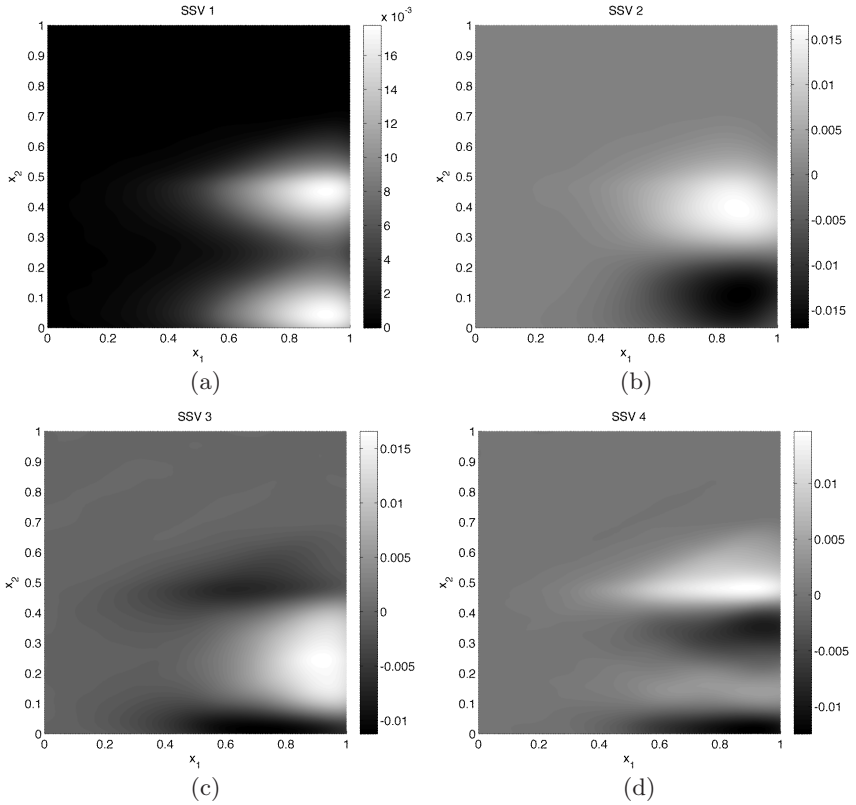


FIGURE 4. The first four spatial sensitivity vectors.

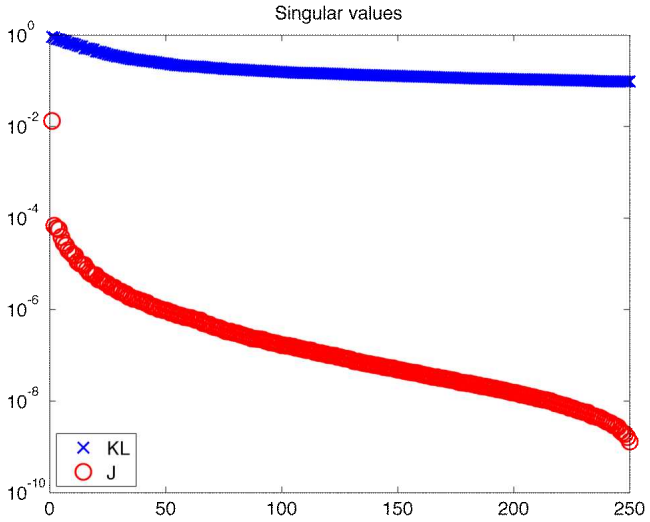


FIGURE 5. Singular values of the Karhunen-Loeve expansion (x) compared to the singular values of the matrix J (circle).

REFERENCES

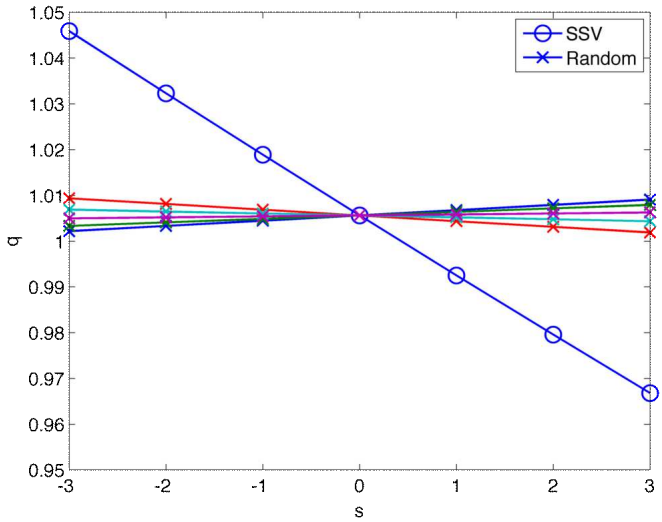


FIGURE 6. The quantity of interest q along the dominant SSV compared to random normalized directions in the space of ξ. The parameter s on the horizontal axis scales the normalized directions. One can clearly see that changes along the SSV have greater impact on the quantity of interest.

CHEN, H., WANG, Q., HU, R. & CONSTANTINE, P. 2011 Conditional sampling and experiment design for quantifying manufacturing error of a transonic airfoil. *AIAA-2011-658* .

CONSTANTINE, P. G. & WANG, Q. 2012 Input subspace detection for dimension reduction in high-dimensional approximation. *arXiv:1202.3508* .

SALTELLI, A., RATTO, M., ANDRES, T., CAMPOLONGO, F., CARIBONI, J., GATELLI, D., SAISANA, M. & TARANTOLA, S. 2008 *Global Sensitivity Analysis. The Primer*. John Wiley & Sons, Ltd.