

Surrogate modeling for sensitivity analysis of models with high-dimensional outputs

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ABSTRACT: Sensitivity analysis provides important information on how the input uncertainty impacts the system output uncertainty. Typically, sensitivity analysis entails large number of system evaluations. For expensive system models with high-dimensional outputs, direct adoption of such models for sensitivity analysis poses significant computational challenges. To address these challenges, an efficient dimension reduction and surrogate based approach is proposed for efficient sensitivity analysis of expensive system models with high-dimensional outputs. As an example, the proposed approach is applied to investigate the sensitivity of peak water level over large coastal regions in San Francisco Bay with respect to the construction of levees at different counties under projected sea level rise.

1. INTRODUCTION

Sensitivity analyses have a prominent role in probabilistic studies, aiming to quantify the impact of the uncertain inputs on the system model outputs (Saltelli, 2002). Evaluation of each sensitivity index typically requires a separate Monte Carlo simulation (MCS) (Sobol', 2001) with many evaluations of the system model, which creates huge challenges for applications involving computationally expensive models. To reduce the computational burden, researchers have investigated alternative frameworks for approximating sensitivity indices, for example, the adoption of metamodel-based approaches (Oakley and O'Hagan, 2004; Sudret, 2008; Le Gratiet et al., 2017; Nagel et al., 2018). However, most of the surrogate model-based approaches for sensitivity analysis focus on scalar outputs and may not be suitable for sensitivity analysis of models with high-dimensional outputs. For

system models with high-dimensional outputs, if building a surrogate model for each output, the computational effort to train the surrogate models for all the outputs and then subsequently use them for prediction and sensitivity analysis will be huge. Also, the use of MCS for estimation of Sobol' indices in this context may entail significant memory requirements considering the need to use large number of samples for the inputs and the need to store the corresponding high-dimensional outputs for each of the samples. Recently Marelli and Sudret (2015) proposed a compressive polynomial chaos expansions (PCE) for multi-dimensional model maps where a two-state PCE is developed to address some of above challenges and calculate stochastic properties of the high-dimensional outputs.

To facilitate global sensitivity analysis of expensive models with high-dimensional outputs, this pa-

per proposes an efficient dimension reduction and surrogate based approach for sensitivity analysis of expensive models with high-dimensional outputs. This approach is named as Dimension REduction and Surrogate based Sensitivity Analysis (DRE-SSA). DRE-SSA establishes a kriging surrogate model to address the computational challenge in repeated evaluations of the expensive model for sensitivity analysis. In this context, to address the challenge of building surrogate model for high-dimensional outputs, DRE-SSA uses Principal Component Analysis (PCA) to establish a low-dimensional latent output representation. The surrogate model is then conveniently built for the low-dimensional latent output. For sensitivity analysis, DRE-SSA first uses surrogate model in latent space to efficiently calculate the relevant covariance matrices for the latent outputs, which requires significantly less computational effort and memory requirements. Then, DRE-SSA directly establishes the sensitivity indices for the original high-dimensional output based on the derived relationship between these sensitivity indices and the established covariance matrices for the latent outputs. As an example, the proposed approach is applied to calculate sensitivity indices for peak water level (PWL) over large coastal regions in San Francisco (SF) Bay with respect to the construction of levees at different counties along the shoreline under projected sea level rise (SLR).

2. SENSITIVITY ANALYSIS FOR EXPENSIVE MODELS WITH HIGH DIMENSIONAL OUTPUTS

In this paper, we will discuss sensitivity analysis for expensive models with high-dimensional outputs using Sobol' index (which is a commonly used variance-based global sensitivity measure) as the sensitivity measure. Consider a system model with uncertain model parameters representing the system input $\mathbf{x} = [x_1, \dots, x_i, \dots, x_{n_x}]^T$ where x_i is the i^{th} input and n_x is the total number of inputs, let $\mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), \dots, y_k(\mathbf{x}), \dots, y_{n_y}(\mathbf{x})]$ denote the corresponding system outputs where for high-dimensional outputs n_y will be large number. Now we consider the sensitivity for each output y_k . Take the first order Sobol' index for example, let $S_{k,i}^y$ denote the first

order Sobol' index of the k^{th} output y_k with respect to the i^{th} input x_i , then $S_{k,i}^y$ can be written as

$$S_{k,i}^y = \frac{V_{k,i}^y}{V_k^y} = \frac{\text{Var}_i [E_{\sim i} (y_k(\mathbf{x})|x_i)]}{\text{Var} [y_k(\mathbf{x})]} \quad (1)$$

where $E_{\sim i}[\cdot]$ represents the expectation with respect to $\mathbf{x}_{\sim i}$, which corresponds to all inputs excluding x_i .

We need to calculate $S_{k,i}^y$ for each $k = 1, \dots, n_y$ and $i = 1, \dots, n_x$. In the end, the sensitivity information for all outputs with respect to all the inputs can be represented by a sensitivity index matrix \mathbf{S}^y of dimension $n_y \times n_x$. Evaluation of $S_{k,i}^y$ requires knowledge of $\text{Var}_i [E_{\sim i} (y_k(\mathbf{x})|x_i)]$ in the numerator, which involves a double loop integration. For evaluating the Sobol' indices, the most generalized approach is Monte Carlo Simulation (MCS) (Sobol', 2001). However, this typically entails large number of evaluations of the system model. For example, suppose N samples (typically N is large number) are used for MCS, this approach would require $N \times n_x$ model evaluations to obtain all first order indices $S_{k,i}^y$. To obtain higher order indices, more model evaluations are needed. Apparently, direct adoption of the expensive model within MCS for sensitivity analysis will be computationally prohibitive. Besides the computational effort, calculating the sensitivity index for all the outputs in the context of MCS may also entail significant memory requirements considering the need to use large number of samples and the need to store the corresponding high-dimensional outputs for each of the samples.

3. DIMENSION REDUCTION AND SURROGATE BASED SENSITIVITY ANALYSIS OF EXPENSIVE MODELS WITH HIGH-DIMENSIONAL OUTPUTS

To address the above challenges and facilitate global sensitivity analysis of expensive models with high-dimensional outputs, this paper proposes an efficient dimension reduction and surrogate based approach for sensitivity analysis. This approach is named as Dimension REduction and Surrogate based Sensitivity Analysis (DRE-SSA). The flowchart for the overall approach is shown in Figure 1.

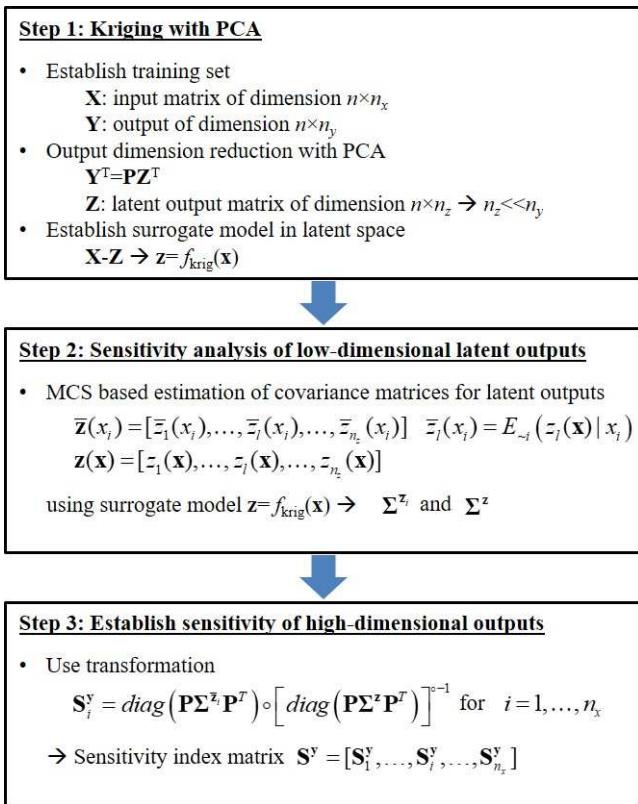


Figure 1: Flowchart for the proposed DRE-SSA method for sensitivity analysis of expensive models with high-dimensional outputs.

Specifically, to address the computational challenge in repeated evaluation of the expensive system model, a kriging surrogate model is established in place of the expensive model for use in MCS-based estimation of sensitivity indices. Instead of building kriging for the high-dimensional outputs, Principal Component Analysis (PCA) is adopted to establish a low-dimensional latent outputs representation and the surrogate model is built with respect to the low-dimensional latent outputs. For sensitivity analysis, it is first carried out efficiently for the low-dimensional latent outputs Jia and Taflanidis (2013); Blatman and Sudret (2013). Then, the sensitivity indices of the original high-dimensional output are directly established using the derived transformation from latent space to original space. Overall, the proposed approach allows efficient calculation of the sensitivity indices of expensive models with high-dimensional outputs. The following sections discuss in detail the steps of the proposed approach.

3.1. Kriging with PCA

3.1.1. Training set

To build the surrogate model, we first run n evaluations of the expensive system model. We will have the output vector $\{\mathbf{y}^h = \mathbf{y}(\mathbf{x}^h); h = 1, \dots, n\}$ for each input $\{\mathbf{x}^h; h = 1, \dots, n\}$. We will denote by $\mathbf{X} = [\mathbf{x}^1, \dots, \mathbf{x}^n]^T \in R^{n \times n_x}$ and $\mathbf{Y} = [\mathbf{y}^1, \dots, \mathbf{y}^n]^T \in R^{n \times n_y}$ the corresponding input and output matrices, respectively, which form the training set.

3.1.2. Output dimension reduction by PCA

PCA finds a low-dimensional representation of the high-dimensional data. The corresponding low-dimensional outputs are typically called principal components or latent outputs. The latent output matrix of size $n \times n_z$ can be established through the transformation

$$\mathbf{Y}^T = \mathbf{PZ}^T \quad (2)$$

where \mathbf{P} is the $n_y \times n_z$ projection matrix. The value of n_z can be chosen so that latent outputs account for at least r_o [say 99%] of the total variance of the data in \mathbf{Y} (Tipping and Bishop, 1999). Typically, $n_z \ll n_y$, leading to a significant reduction in the output dimension. Essentially, the transformation in Eq. (2) can be used to transform latent outputs to original outputs. Let $\mathbf{z} = [z_1, \dots, z_l, \dots, z_{n_z}]$ denote the vector of latent outputs, we have $\mathbf{y}^T = \mathbf{Pz}^T$.

3.1.3. Surrogate model in latent space

Due to the low dimensionality of the latent outputs \mathbf{z} , a single kriging surrogate model can be built with respect to each of the latent outputs in \mathbf{z} (?). Take the l^{th} latent output for example, based on the set of n observations with input matrix \mathbf{X} and corresponding latent output \mathbf{Z}_l (i.e., l^{th} column of \mathbf{Z}), kriging establishes an approximation to $z_l(\mathbf{x})$, denoted $\hat{z}_l(\mathbf{x})$, for any new input \mathbf{x} through (Sacks et al., 1989)

$$\hat{z}_l(\mathbf{x}) = \mathbf{f}_l(\mathbf{x})^T \alpha_l^* + \mathbf{r}_l(\mathbf{x})^T \beta_l^* \quad (3)$$

where $\alpha_l^* = (\mathbf{F}_l^T \mathbf{R}_l^{-1} \mathbf{F}_l)^{-1} \mathbf{F}_l^T \mathbf{R}_l^{-1} \mathbf{Z}_l$ and $\beta_l^* = \mathbf{R}_l^{-1} (\mathbf{Z}_l - \mathbf{F}_l \alpha_l^*)$ are coefficient vectors. Here $\mathbf{f}_l(\mathbf{x})$ is the n_p -dimensional basis vector, and $\mathbf{F}_l = [\mathbf{f}_l(\mathbf{x}^1) \dots \mathbf{f}_l(\mathbf{x}^n)]^T$ is the $n \times n_p$ basis matrix. \mathbf{R}_l is the $n \times n$ correlation matrix with the jk^{th} element

defined as $R(\mathbf{x}^j, \mathbf{x}^k)$ (e.g., one commonly used correlation function is the generalized exponential correlation). Through tuning the parameters of the correlation function, kriging can efficiently approximate very complex functions. The optimal selection of \mathbf{s} is typically based on the Maximum Likelihood Estimation (MLE) principle (Lophaven et al., 2002).

Based on the prediction in latent space, the predictor for $\mathbf{y}(\mathbf{x})$ can be established as $\hat{\mathbf{y}}(\mathbf{x})^T = \mathbf{P}\hat{\mathbf{z}}(\mathbf{x})^T$. To assess the surrogate model accuracy, we use the relative mean absolute error (relative MAE, also known as the Mean Absolute Deviation Percent or MADP) for the original outputs \mathbf{y} . For this purpose, a leave-one-out cross validation (LOOCV) is used (?). The MADP for the k^{th} output is calculated as

$$MADP_k = \frac{\sum_{h=1}^n |y_k(\mathbf{x}^h) - \hat{y}_k(\mathbf{x}^h)|}{\sum_{h=1}^n |y_k(\mathbf{x}^h)|} \quad (4)$$

Smaller values for $MADP_k$ (closer to zero) indicate a good fit. Further, the average MADP (AMADP) over all output dimensions can be established as well, $AMADP = \sum_{k=1}^{n_y} MADP_k / n_y$.

3.2. Sensitivity analysis for high-dimensional outputs

In this section, we derive the relationship between sensitivity of the high-dimensional original outputs with respect to the inputs and sensitivity (or more specifically the covariance matrices) of the much lower-dimensional latent outputs with respect to the inputs. Take the first order Sobol' index for example, we are interested in the sensitivity index matrix \mathbf{S}^y and we need to calculate $S_{k,i}^y$ for each $k = 1, \dots, n_y$ and $i = 1, \dots, n_x$. Let $\bar{y}_k(x_i)$ represent $E_{\sim i}(y_k(\mathbf{x})|x_i)$, and based on the definition of $S_{k,i}^y$, we need to calculate $V_{k,i}^y$ and V_k^y , corresponding to the variance of $\bar{y}_k(x_i)$ and $y_k(\mathbf{x})$, respectively. Similarly for the latent outputs, we will use the notation $\bar{z}_l(x_i) = E_{\sim i}(z_l(\mathbf{x})|x_i)$. Based on the transformation $\mathbf{y}(\mathbf{x})^T = \mathbf{P}\mathbf{z}(\mathbf{x})^T$ between the high-dimensional original outputs and the low-dimensional latent outputs, we can express the variances of $\bar{y}_k(x_i)$ and $y_k(\mathbf{x})$ in terms of the variances of the latent outputs $\bar{\mathbf{z}}_i = \bar{\mathbf{z}}(x_i) = [\bar{z}_1(x_i), \dots, \bar{z}_l(x_i), \dots, \bar{z}_{n_z}(x_i)]$ and $\mathbf{z} = \mathbf{z}(\mathbf{x}) = [z_1(\mathbf{x}), \dots, z_l(\mathbf{x}), \dots, z_{n_z}(\mathbf{x})]$, respectively. More specifically, let Σ^z denote the

$n_z \times n_z$ covariance matrix for the latent outputs $\mathbf{z}(\mathbf{x})$, and $\Sigma^{\bar{z}_i}$ denote the $n_z \times n_z$ covariance matrix for $\bar{\mathbf{z}}(x_i)$. The covariance matrices of $\bar{\mathbf{y}}_i = \bar{\mathbf{y}}(x_i) = [\bar{y}_1(x_i), \dots, \bar{y}_k(x_i), \dots, \bar{y}_{n_y}(x_i)]$ and $\mathbf{y} = \mathbf{y}(\mathbf{x}) = [y_1(\mathbf{x}), \dots, y_k(\mathbf{x}), \dots, y_{n_y}(\mathbf{x})]$, can be written as

$$\Sigma^{\bar{y}_i} = \mathbf{P}\Sigma^{\bar{z}_i}\mathbf{P}^T \quad (5)$$

and

$$\Sigma^y = \mathbf{P}\Sigma^z\mathbf{P}^T \quad (6)$$

respectively, where the interested variances $\mathbf{V}_i^y = [V_{1,i}^y, \dots, V_{k,i}^y, \dots, V_{n_y,i}^y]^T$ and $\mathbf{V}^y = [V_1^y, \dots, V_k^y, \dots, V_{n_y}^y]^T$ correspond to the diagonal elements of $\Sigma^{\bar{y}_i}$ and Σ^y , respectively. Then based on the definition of sensitivity index in Eq. (1), we can write the i^{th} column of \mathbf{S}_i^y , which corresponds to the sensitivity index of all the outputs with respect to the i^{th} input x_i , as

$$\mathbf{S}_i^y = diag(\mathbf{P}\Sigma^{\bar{z}_i}\mathbf{P}^T) \circ [diag(\mathbf{P}\Sigma^z\mathbf{P}^T)]^{\circ -1} \quad (7)$$

where $diag(\cdot)$ denotes the diagonal operator and establishes a vector consisting of the diagonal elements of a matrix. The notation $A \circ B$ means the Hadamard product of matrix A and B , i.e., elementwise product, and $B^{\circ -1}$ means the Hadamard inverse of matrix B , i.e., elementwise inverse. Note that sensitivity indices for higher order interactions can be established similarly.

From Eq. (7), we can see that to calculate \mathbf{S}_i^y (for $i = 1, \dots, n_x$), we can first calculate the covariance matrices $\Sigma^{\bar{z}_i}$ (for $i = 1, \dots, n_x$) and Σ^z , and then use the transformation in Eq. (7) to establish the sensitivity index for the original high-dimensional outputs. These covariance matrices (i.e., $\Sigma^{\bar{z}_i}$ and Σ^z) can be estimated using the established kriging surrogate model $\hat{\mathbf{z}}(\mathbf{x})$ for the latent outputs $\mathbf{z}(\mathbf{x})$ and MCS. Due to the high efficiency of surrogate model and the low-dimensionality of the latent outputs, these covariance matrices can be established with high efficiency and low memory requirements.

4. ILLUSTRATIVE EXAMPLE

As an illustrative example, the proposed DRE-SSA method is applied to investigate how the construction of containments (such as levees, seawalls) at

different locations around SF Bay would impact the peak water level (PWL) over the entire SF Bay region under projected SLR, which is formulated as a sensitivity analysis problem. The application of DRE-SSA facilitates efficient sensitivity analysis, considering the fact that the high-fidelity numerical model for the hydrodynamics of SF Bay is computationally expensive and the interested outputs (i.e., PWL over the entire SF Bay) corresponds to extremely high-dimensional outputs. In the end, sensitivity maps useful for guiding decision making are generated for first order main effects using the proposed DRE-SSA method.

4.1. Sensitivity analysis

Here the decision of whether to build a containment at each county along SF Bay is treated as input to the numerical model, i.e., $\mathbf{x} = [x_1, \dots, x_i, \dots, x_{n_x}]^T$ with $n_x = 8$ where x_i for $i = 1, \dots, n_x$ corresponds to Marin County, Sonoma County, Napa County, Solano County, Contra Costa County, Alameda County, Santa Clara County, and San Mateo County, respectively. We artificially treat each component x_i in \mathbf{x} as uncertain with uniform distribution in $[0, 1]$. $x_i < 0.5$ means that the i^{th} containment will not be constructed, and $x_i \geq 0.5$ means that the i^{th} containment will be constructed. For the output $\mathbf{y} = \mathbf{y}(\mathbf{x})$, we are interested in the PWL at each location in the computational domain, i.e., $\mathbf{y} = [y_1, \dots, y_k, \dots, y_{n_y}]$ with $n_y = 80,050$ in the current example.

4.2. High-fidelity database for surrogate modeling

To establish the database for building surrogate model, we generate n inputs. To generate inputs that can uniformly span the entire input space, which is desirable for building surrogate model with good accuracy over the input space, we use Sobol low-discrepancy sequence. This in the end gives the input matrix \mathbf{X} . Then the high-fidelity model is evaluated for each of the n inputs, the PWL is obtained for all locations, giving the corresponding output matrix \mathbf{Y} with dimension $n \times n_y$. For the projected SLR, we used the case of 1.5m.

For the high-fidelity model, we used Delft3D Flow Flexible Mesh (D-Flow FM) to accurately

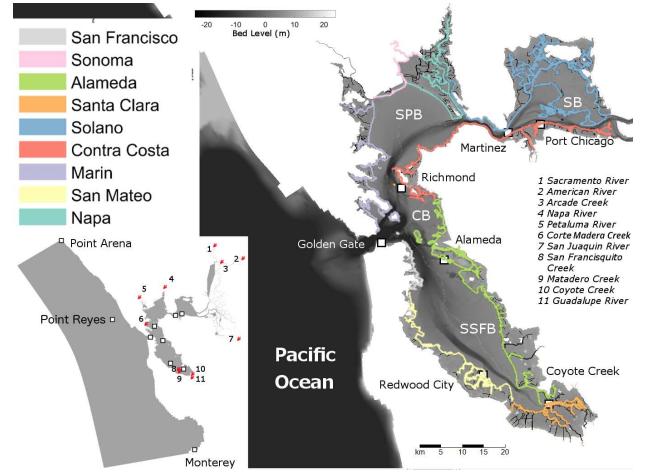


Figure 2: The computational domain covers SF Bay and an open ocean area. The color line represents the position of the seawalls at different counties.

simulate the tidal dynamics of SF Bay. This software solves the shallow-water equation using an unstructured grid. The resolution we used here is up to the scale of 50 m close to the shoreline, allowing us to more accurately resolve the coastal infrastructure and other flood-control features. Levee structures were simulated using the empirical “fixed weir” model at the corresponding counties if $x_i \geq 0.5$. An open boundary condition was applied outside of the Golden Gate. The model included 11 river discharges imposed at the numbered locations in Figure 2. A drying and wetting numerical scheme was applied to the intertidal region. More details about the model can be found in Wang et al. (2017). The established high-fidelity numerical model can accurately simulate the water level over the entire bay region under different containment locations and SLR scenarios. Each simulation of this high-fidelity numerical model takes around 20 hours.

5. RESULTS AND DISCUSSIONS

5.1. Implementation details of DRE-SSA

For the dimension of latent outputs for PCA, the selection of $r_o = 99.9\%$ leads to $n_z = 20$. For the number of samples in the training set, considering the high computational effort for each evaluation of the high-fidelity model, it is desirable to use small number for n as long as the established kriging surrogate model reaches the targeted accuracy. Fig-

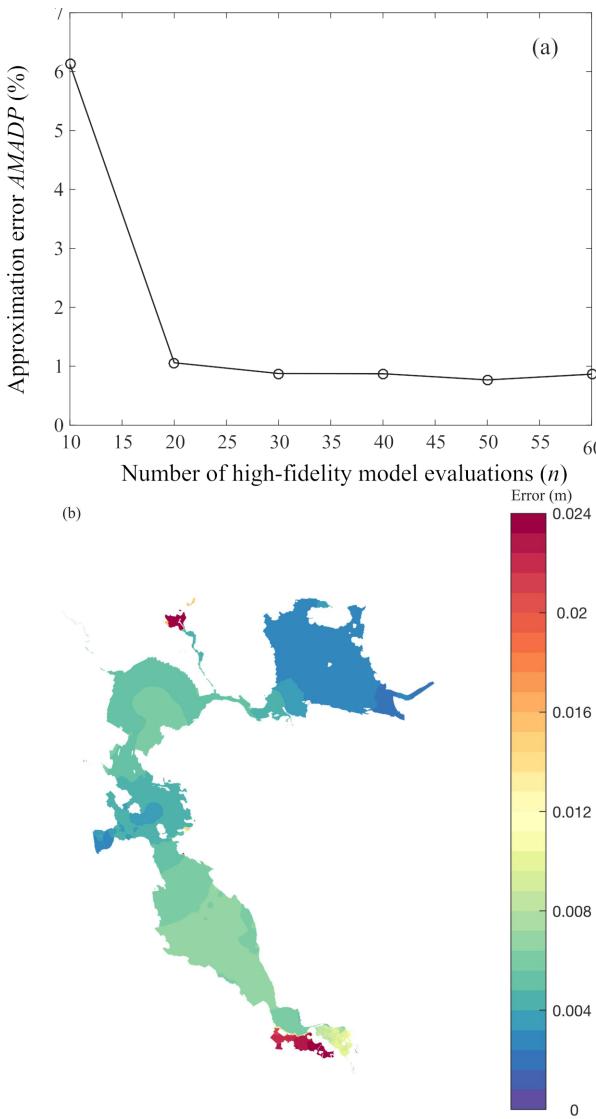


Figure 3: Accuracy of the established kriging surrogate model, (a) variation of kriging accuracy with the number of high-fidelity evaluations, (b) approximation error over all outputs

Figure 3(a) shows how the approximation error, measured by $AMADP$, changes over different selection of n . For the analysis, when n is larger than 40, there is little variation in the error and the $AMADP$ is below 1%, indicating good accuracy of the established kriging surrogate model. Therefore, we use $n = 40$ and $n_z = 20$ for building kriging with PCA and subsequent sensitivity analysis. To further illustrate the accuracy of the established kriging surrogate model, the error $MADP_k$ for each location is calculated and plotted in Figure 3(b). As can be seen the established kriging model provides good

accuracy with small error over the entire computational domain.

To calculate the covariance matrices for the latent outputs, MCS is used where kriging surrogate model is used for prediction of latent outputs $\mathbf{z}(\mathbf{x})$ for any \mathbf{x} . To establish accurate estimation of the covariance matrices and ultimately the sensitivity indices, $N=100,000$ samples are used in MCS. Once the covariance matrices are established, we use the transformation in Eq. (7) to establish the sensitivity index matrix \mathbf{S}^y for the original high-dimensional outputs. Since each of the output dimension corresponds to a spatial location in the computational domain, we can generate sensitivity maps for each input x_i to help visualize \mathbf{S}^y .

5.2. Performance of DRE-SSA

To validate DRE-SSA, the sensitivity indices calculated by DRE-SSA are compared with the ones calculated from directly building surrogate models for each of the high-dimensional outputs (with the latter referred as SSA). For the purpose of validating the derived transformations, the results from SSA can be taken as the accurate reference values. As an illustration, Figure 4 shows the sensitivity maps for the first order main effects of Napa County calculated by DRE-SSA and SSA. The R^2 value is around 0.994 considering sensitivity index predictions at all locations plotted on the map. As can be seen, the DRE-SSA has good accuracy and can accurately estimate sensitivity indices for models with high-dimensional outputs.

However, it is important to note that there are several sources of errors in DRE-SSA, namely (i) truncation error in PCA, (ii) error in surrogate model, and (iii) error from MCS. By selecting a large value for r_o (e.g., $r_o = 99.9\%$), the truncation error by PCA will typically be extremely small and can be neglected. The error from MCS can be reduced by increasing the number of simulations. The adoption of surrogate model allows efficient implementation of MCS with large number of simulations. Therefore, these two sources of error can be easily reduced. On the other hand, the error from surrogate model can be reduced by using larger number of samples in the training set either through directly using techniques such as Latin Hy-

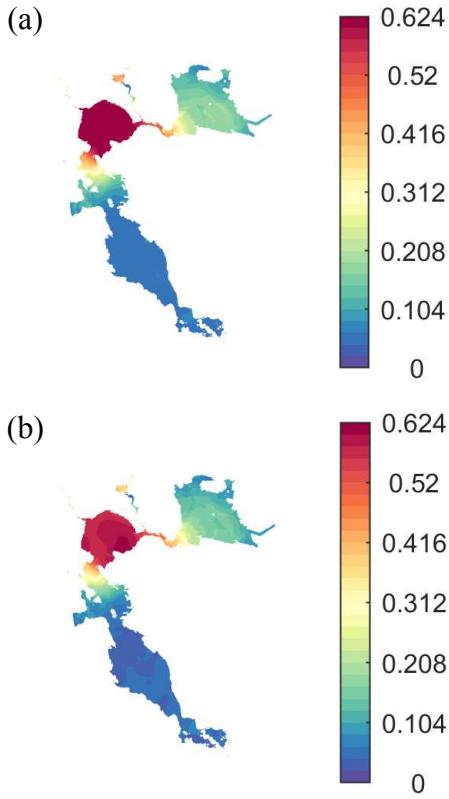


Figure 4: Sensitivity map for first order main effect of Napa County by (a) DRE-SSA and (b) SSA.

percube Sampling (LHS) or adaptive selection of new samples to add into the existing training set. In the current example, by using $r_o = 99.9\%$ for PCA, $N=100,000$ samples for MCS, and selecting $n=40$ to establish surrogate model with *AMADP* below 1%, the overall error in the sensitivity index estimation is expected to be small. Future work will investigate how to explicitly incorporate these errors in the sensitivity index estimation, especially for cases when some of the errors are not so small to be neglected.

5.3. Sensitivity maps

Figure 4 already showed the sensitivity map with respect to the construction of containments at Napa County. Figure 5 shows the sensitivity maps for the first order main effects for several other inputs. More specifically, Figure 4 shows that the construction of containments at Napa County will have relatively large impact on the variation of PWL in the San Pablo Bay (SPB) region while having small im-

pact on the PWL of the rest of the bay.

Figure 5(a) shows that the construction of containments at Solano County will have localized impacts on the PWL, with large impact on northern parts of Suisun Bay (SB) but relatively small impact on the PWL of the rest of the bay. Figure 5(b) shows that the construction of containments at San Mateo County will have relatively large impact on the variation of PWL in the entire bay with the most prominent impact happening at Central Bay (CB). The above information (along with sensitivity maps for all the other inputs) can be used to guide decision making regarding construction of containment or not at a specific county.

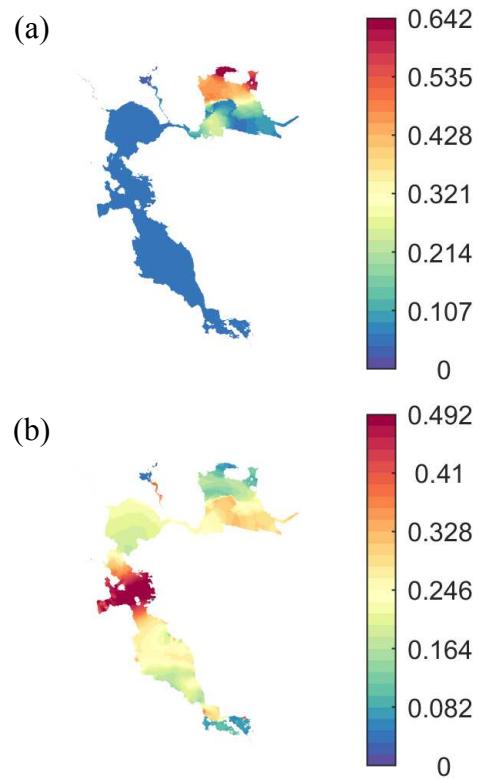


Figure 5: Sensitivity map for first order main effects of (a) Solano County, and (b) San Mateo County.

6. CONCLUSIONS

This paper proposed an efficient dimension reduction and surrogate based approach for global sensitivity analysis of expensive models with high-dimensional outputs. The proposed DRE-SSA uses surrogate model to address the computational

challenge in repeated evaluations of the expensive model for sensitivity analysis and uses PCA as the dimension reduction technique to establish a low-dimensional latent output representation of the original high-dimensional outputs to address the challenge of building surrogate model for high-dimensional outputs. For sensitivity analysis, the relevant covariance matrices are first carried out efficiently for the latent outputs using surrogate model, and then this information is used in the derived transformation to directly establish the sensitivity indices for the original high-dimensional output. Overall, the proposed approach allows efficient calculation of the sensitivity indices of expensive models with high-dimensional outputs. Results from the illustrative example verified the performance and accuracy of the DRE-SSA method. The generated sensitivity maps provide insights on how the construction of levees at different counties would impact PWL over the entire SF Bay.

The proposed approach is general and can be easily applied to sensitivity analysis for other expensive models with high-dimensional outputs and also for calculation of Sobol' indices for total effects and higher order interactions. Although the formulation is presented in the context of using kriging as the surrogate model, other surrogate models can be used as well. While other dimension reduction techniques besides PCA can be used as well, the attractive feature of PCA is that it is a linear transformation, which facilitates the transformation of outputs and corresponding variances between latent outputs and original outputs. More research is still needed in how to explicitly quantify and incorporate the several sources of errors in the sensitivity index estimation.

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