

Surrogate models based on sparse estimation for geotechnical reliability analysis

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ABSTRACT

This paper presents a method for building surrogate models for geotechnical reliability analysis based on sparse estimation. Sparse estimation, which is called least absolute shrinkage statistical operator (lasso) in statistics, has the property that some of the parameters in surrogate models are driven to zero and leads to simpler models. Building surrogate models can be divided into two processes, model selection and parameter estimation, and the sparse estimation enables to achieve these two processes at the same time. A surrogate model was designed to estimate consolidation settlement value of a specific time based on sparse estimation, and its applicability has been investigated by comparing the results by the surrogate model with those by finite element analysis.

Keywords: reliability analysis; surrogate models; lasso; consolidation settlement

1 INTRODUCTION

Surrogate models, also called “response surface” or “meta models”, are regression equations approximate relationships between input and output data in numerical simulations and have been commonly used for parameter identifications and reliability analysis in many research fields. Applications of surrogate models to civil engineering include Bucher and Bourgund (1990), Tandjiria et al. (2000), Youssef and Soubra (2008), Schoefs et al. (2013), and Zhang et al. (2015)

Building surrogate models can be divided into two problems, model selection and parameter estimation. Model selection problems include choice of basis functions and the determination of the model complexity, whereas parameter estimations include determining coefficients of the basis functions. All possible combinations of basis functions and their coefficients should be analyzed to build the “best” surrogate model. This problem, however, is difficult to solve because the time to find a solution grows exponentially with problem size and is known as “NP-hard” problem. The methodology to efficiently achieve model selection and coefficient estimation is necessary for building more accurate surrogate models.

This study proposes an efficient method for building surrogate models based on sparse estimation. The proposed method enables to efficiently solve model selections and parameter estimations at the same time. The applicability of the surrogate models based on the proposed method was investigated through numerical examples of geotechnical reliability analysis, and the results are compared with those by existing method.

2 SURROGATE MODELS BASED ON SPARSE ESTIMATION

We use M^{th} order polynomial functions as surrogate models for simplicity. When the input parameter is x , the polynomial function f is defined by:

$$f = w_0 + w_1x + w_2x^2 + \dots + w_Mx^M = \sum_{j=0}^M w_jx^j \quad (1)$$

where, w_0, \dots, w_M are polynomial coefficients.

The values of the coefficients will be determined by fitting the polynomial function to the training data y_n . This fitting is usually done by minimizing the least squares objective function:

$$J(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{f(x, \mathbf{w}) - y_n\}^2 \quad (2)$$

where N is the number of training data. When the squared error between the model predictions and training data follows Gaussian distribution and the model function is linear, the analytical solution can be obtained using the least square method.

2.2 Regularization

There remains the problem of choosing the order M of the polynomial, and this is an example of “model selection”. Lower order polynomials, $M = 0$ and 1, give poor fits to the data, and higher order polynomials generally give good fits to the data. When we define $M = N$, the polynomial passes exactly through each data point and the objective function equals 0.

There is a technique that is often used to control over-fitting phenomenon in such cases is that of regularization, which involves adding a penalty term to the objective functions to discourage the coefficients from reaching large values. The general expression of the modified objective functions including regularization term takes the form

$$\tilde{J}(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{f(x, \mathbf{w}) - y_n\}^2 + \frac{\lambda}{2} \sum_{j=1}^M |w_j|^q \quad (3)$$

where λ is the regularization parameter which governs the relative importance of the regularization term compared with the sum-of-squares effort term, q is the parameter controls the regularization term, and $q = 2$ corresponds to the quadratic regularizer, so-called Ridge regression, which is defined by

$$\tilde{J}_R(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{f(x, \mathbf{w}) - y_n\}^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2 \quad (4)$$

where $\|\mathbf{w}\|^2 = \mathbf{w}^T \mathbf{w} = w_0^2 + w_1^2 + \dots + w_M^2$.

The case of $q = 1$ is called least absolute shrinkage statistical operator (lasso, Tibshirani 1996), and it takes the form.

$$\tilde{J}_L(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^N \{f(x, \mathbf{w}) - y_n\}^2 + \frac{\lambda}{2} |\mathbf{w}| \quad (5)$$

where $|\mathbf{w}| = |w_0| + |w_1| + \dots + |w_M|$. It has the property that if λ is sufficiently large, some of the coefficients w_j are driven to zero because of the geometry of its regularization term. Figure 1 illustrates the estimation graph of ridge regression and the lasso, and x_1 becomes zero because of the diamond-shaped regularization term. The lasso tends to lead to a sparse model in which the corresponding basis functions play no role. Estimating for surrogate models via the lasso is called “sparse estimation” in this paper.

2.3 Algorithm for Sparse Estimation

The lasso problem is a convex minimization problem, a quadratic program with a convex constraint. For simplicity, the following problem is used to explain the computational procedure for the lasso solution.

$$\underset{w}{\text{minimize}} \left\{ \frac{1}{2} (w - y_n)^2 + \frac{\lambda}{2} |w| \right\} \quad (6)$$

The standard approach to this one-dimensional minimization problem is to take the gradient with respect to w and to set it to zero. However, one of the central difficulties in solving Equation (6) is the presence of a non-smooth L1 norm, $|w|$. In other words, the absolute value function $|w|$ does not have a derivative at $w = 0$. Nevertheless, this problem can be solved by applying a soft-thresholding operator to w , which is defined as

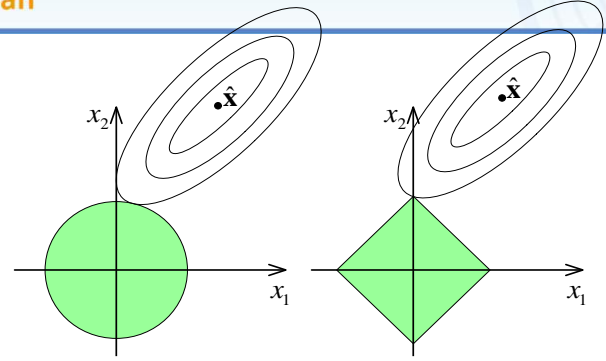


Fig. 1. Estimation picture for ridge (left) and lasso (right) regression (modified from Hastie et al. 2015).

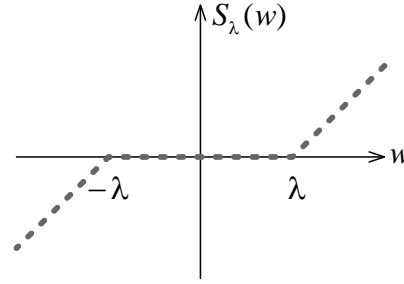


Fig. 2. Soft-thresholding function.

$$S_\lambda(w) = \begin{cases} w - \lambda & (w > \lambda) \\ 0 & (-\lambda \leq w \leq \lambda) \\ w + \lambda & (w < -\lambda) \end{cases} \quad (7)$$

where S_λ is a soft-thresholding function (Fig. 2). This operator translates w toward zero by an amount λ and sets it to zero if $|w| < \lambda$. When $\lambda = 0$, the solution of Equation (5) becomes the solution for the ordinary least squares problem. The general approach for solving the lasso problem can be summarized as follows:

- Step 1: Minimize first term in the objective function
- Step 2: Apply the soft-thresholding operator to w
- Step 3: Repeat Steps 1 and 2

To minimize the lasso-type objective function, we used Alternative Direction Method of Multipliers (ADMM, Boyd et al., 2010).

3 APPLICATION EXAMPLES

3.1 Setup

We built a surrogate model to estimate a value of ground surface settlement due to embankment loading. This section presents the setup of the numerical example.

Figs. 3 (a) and (b) show the model ground discretized with finite element mesh and the construction process of the embankment. The model ground is assumed to consist of three layers (sand layer, clay layer, and sandy clay), and the layers were modeled as an linear elastic model and Cam-clay models. An embankment is assumed to be constructed on the model ground following the construction process shown in Fig. 3(b), and time-settlement behavior of the ground is observed

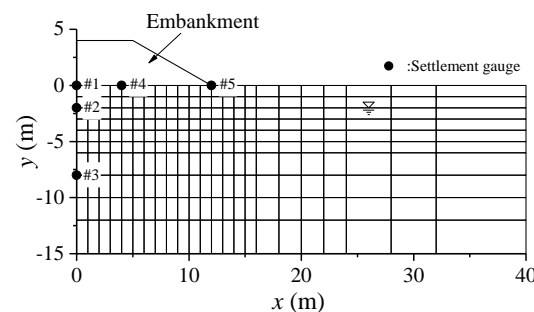
at five points #1 ~ #5.

The surrogate model was designed to estimate the settlement value at #1 after 2,500 days after construction began, and this settlement value is the output (or the objective variable) in the surrogate models. We assumed that ten parameters, elastic modulus E and the Poisson's ratio ν of the sand layer, and the compression index λ_c , the swelling index κ , the critical state parameter M , and the coefficient of permeability k (m/d) of the clay and sandy clay layers, as the input parameters. The total number of input parameters is ten.

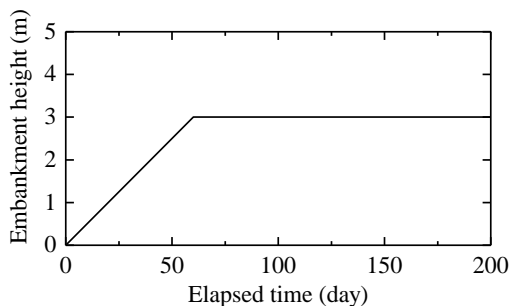
The performance of the surrogate models depends on the value of regularization parameter λ , and we determined the parameter using leave-one-out cross-validation which is commonly and widely used in many research fields. In this study, we built two surrogate models 1) $N = 1,000$ and 2) $N = 50$ to investigate the effect of the number of training data on building surrogate models. The performance of the surrogate model was evaluated by comparing the estimated probability density function of the target settlement value by the surrogate model with the true value, i.e., the PDF by finite element analysis.

3.2 Case 1: $N = 1,000$

$N = 1,000$ was used to build the surrogate model, and the target settlement values were estimated by the lasso-based model and ridge-based model. Fig. 4



(a) Finite element mesh



(b) Embankment loading process.

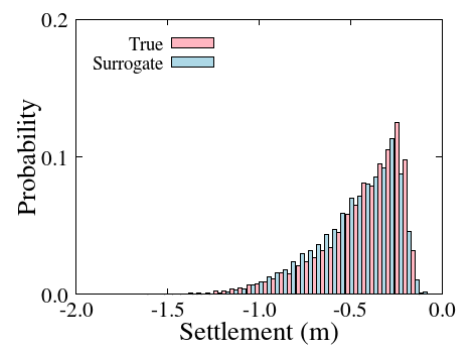
Fig. 3. Setup of numerical simulation.

compares the estimated PDF with the true PDF, and Table 1 summarizes the number of active set and Kullback–Leibler (KL) divergence. The active set

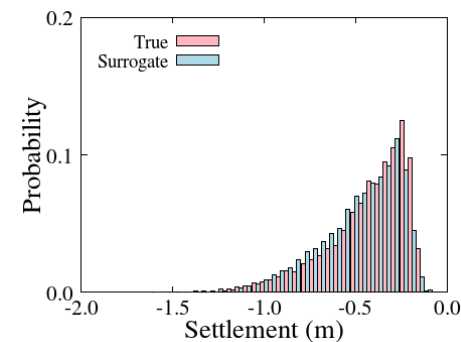
means the number of non-zero components in the solutions, and that number is lower, the simpler surrogate models are built. The KL-divergence is a measure of how one probability distribution is different from a reference probability distribution, and we can quantitatively evaluate the performance of the surrogate models with this measure. The PDF estimated by two methods, lasso and ridge, are very similar and agree well with the true PDF. The KL-divergence of lasso is a bit smaller than that of ridge, and lasso-based model is more accurate than ridge-based model.

3.3 Case 2: $N = 50$

Only 50 data were used to build the surrogate model in Case 2, and this problem is a typical “underdetermined problem” because the number of unknowns is greater than that of observation data. Fig. 5 compares the estimated PDF with the true PDF for ridge and lasso, and Table 2 summarizes the results. The KL-divergence shows that the estimation accuracy of ridge-based model is lower than that of lasso-based model, and the shape of the PDF by ridge is a bit



(a) Ridge regression.



(b) Lasso.

Fig. 4. Comparison of PDF ($N = 1,000$)

Table 1. Summary of Case 1.

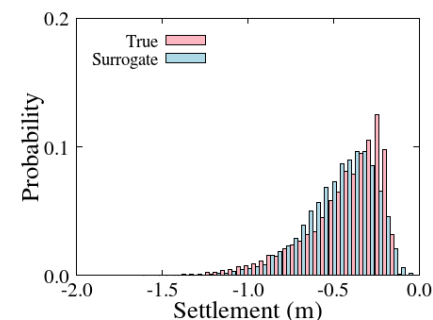
| | Ridge | Lasso |
|---------------------------|---------|---------|
| The number of active sets | 96 | 80 |
| KL-divergence | 0.02672 | 0.02174 |

different from the true PDF. The number of active sets in lasso-based model is 34, and most of the coefficients, 32 input parameters, led to “zero”. Fig. 6(a)(b) shows the solution path of ridge-based and lasso-based

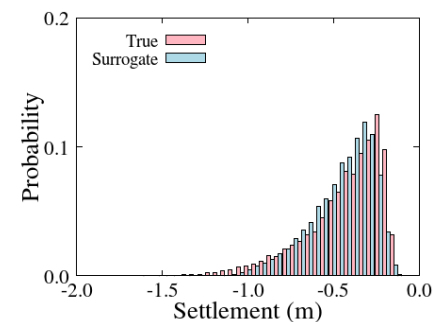
models. The vertical lines indicate the best regularization parameter λ determined by the LOOCV. In ridge regression, regularization parameter is less sensitive to the shrinkage of the coefficients. In lasso, however, the larger λ is used, the simpler model is estimated. These results demonstrate that the proposed lasso-based method for building surrogate models estimate simpler/less complex models and provide more accurate estimations compared to the existing method.

4 CONCLUSIONS

A method for building surrogate models based on lasso was newly proposed. The surrogate model was designed to estimate a value of surface settlement of the ground using the data of the finite element simulations, and the model accuracy was evaluated by comparing the estimated PDF of the settlement value by the surrogate model with the true value, and the result shows that the estimated PDF and the true PDF are in good agreement. The proposed method leads to simpler models compared to the existing method, ridge regression, and the lasso-based model can accurately estimate the PDF with small training data.



(a) Ridge regression.

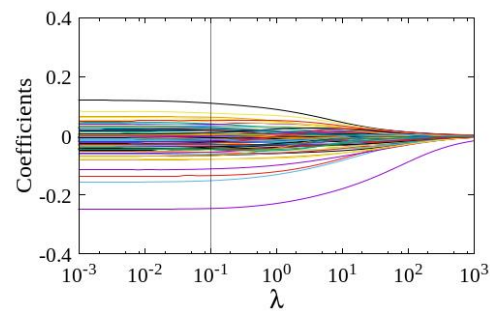


(b) lasso

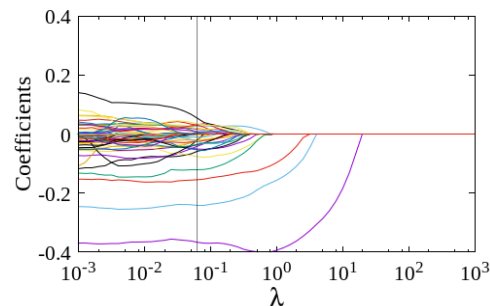
Fig. 5. Setup of numerical simulation.

Table 2. Sizes of margins.

| | Ridge | Lasso |
|---------------------------|---------|---------|
| The number of active sets | 96 | 34 |
| KL-divergence | 0.06578 | 0.03010 |



(c) Ridge regression.



(d) Sparse estimation (lasso).

Fig. 6. Solution path

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