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Robust and reliable metamodels for mechanized tunnel simulations

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ABSTRACT

The main objective of this paper is to construct a robust and reliable metamodel for the mechanized tunnel simulation in computationally expensive applications. To accomplish this, four metamodeling approaches have been implemented and their performance has been systematically evaluated through a comparative study utilizing pure mathematical test functions. These metamodels are quadratic polynomial regression, moving least squares, proper orthogonal decomposition with radial basis functions, and an extended version of the latest approach. This extended version has been proposed by the authors and named proper orthogonal decomposition with extended radial basis functions. After that, a system identification study for mechanized tunneling has been conducted through the back analysis of synthetic measurements. In this study, the best performing metamodel, that is the one suggested by the authors, has been employed to surrogate a complex and computationally expensive 3D finite element simulation of the mechanized tunnel. The obtained results demonstrate that the proposed metamodel can reliably replace the finite element simulation model and drastically reduce the expensive computation time of the back analysis subroutine.

1. Introduction

Most of the advanced geotechnical systems are described through complex mathematical models which cannot be easily solved by analytical approaches. In such cases, numerical techniques such as Finite Element Method (FEM) are used to simulate the responses of the system. During the past decades, along with the significant progresses in computer science, numerical simulations have been established as powerful tools used practically in all fields of engineering and science. In a number of situations, engineering problems require using computationally expensive simulations. Therefore, routine tasks such as design optimization [1], probabilistic studies of uncertainties [2], parameter identification [3–6], inverse problem [7,8] or sensitivity analysis become impossible since they require thousands or even millions of simulations. A common practice for engineers to solve this problem is to develop simplified models to approximate the original model with high level of accuracy. The approximated model which can capture the behavior of the original model is called *metamodel* or *surrogate model.*

Generally, research about metamodeling can be categorized into three groups: (1) papers in which a new metamodeling approach is introduced; see e.g. [8–10], (2) papers which perform comparative study between existing metamodeling approaches; see e.g. [11–14] and (3) papers which apply the metamodeling concept for engineering problems; see e.g. [7,12]. In this paper, first, an introduction to some existing approaches i.e. Polynomial Regression (PR), Moving Least Squares (MLS), and Proper Orthogonal Decomposition with Radial Basis Function (POD-RBF) is presented then a metamodeling approach named Proper Orthogonal Decomposition with Extended Radial Basis Function (POD-ERBF) is formulated. Subsequently, a comparative study is performed. That is, the performance of the selected metamodeling methods is evaluated using different types of purely mathematical functions. Finally, the POD-ERBF approach is applied to a real-world geotechnical problem. A three dimensional tunnel model simulated by finite element method is replaced by the POD-ERBF metamodel. With this simplified model, the inverse analysis of synthetic measurements is carried out to identify the material parameters of the soil around the tunnel.

2. Metamodeling approaches

The main goal of metamodeling is to approximate an unknown function u which describes the behavior of an engineering problem. The only available information is the input and output data in the form of some scattered samples like $(\mathbf{x}, \boldsymbol{u}(\mathbf{x}))$ obtained from

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physical or computational experiments. $\mathbf{x}$ is a vector of s parameters and $\boldsymbol{u}(\mathbf{x})$ is a vector quantity which gives the function value at m observation points. In order to construct a metamodel, two main components are required: (1) *the input parameter matrix* ($\mathbf{P}$) which includes the s parameters of n_p sample points (2) *the matrix of system responses or snapshot matrix* ($\mathbf{U}$) in which the n_p function values of m observation points are recorded. Therefore, $\mathbf{P}$ and $\mathbf{U}$ matrices are of size $s \times n_p$ and $m \times n_p$ respectively. Depending on the structure of $\mathbf{P}$ and $\mathbf{U}$, several techniques for approximating u may be applicable. As mentioned before, in this paper, four metamodeling approaches, including PR, MLS, POD-RBF and an extension of POD-RBF method named POD-ERBF are selected for the comparative study.

2.1. Polynomial regression

Polynomial Regression (PR) is a technique for producing a metamodel using low order polynomials (quadratic or cubic) in a relatively small region of parameter space. In this paper, the approximation function is assumed to be a quadratic polynomial function as below [12–14]:

$$\tilde{u}(\mathbf{x}) = \beta_0 + \sum_{i=1}^{s}\beta_i x_i + \sum_{i=1}^{s}\beta_{ii}x_i^2 + \sum_{i=1}^{s}\sum_{j>i}^{s}\beta_{ij}x_i x_j = \mathbf{X}^T(\mathbf{x})\boldsymbol{\beta}, \tag{1}$$

$$\mathbf{X}^T(\mathbf{x}) = \left[1, x_1, x_2, \ldots, x_s, x_1^2, x_2^2, \ldots, x_s^2, x_1x_2, x_1x_3, \ldots, x_{s-1}x_s\right], \tag{2}$$

$$\boldsymbol{\beta} = [\beta_0, \beta_1, \beta_2, \ldots, \beta_s, \beta_{11}, \beta_{22}, \ldots, \beta_{ss}, \beta_{12}, \beta_{13}, \ldots, \beta_{(s-1)s}]^T, \tag{3}$$

here, x_i is the ith variable of input point $\mathbf{x}$ and s is the number of input parameters or dimension of the input space. Both $\mathbf{X}$ and $\boldsymbol{\beta}$ vectors have $k = (1+s)(2+s)/2$ components [15]. The unknown coefficients $\boldsymbol{\beta}$ are calculated using least square regression. For this reason, the following error function is to be minimized:

$$\mathrm{J} = \sum_{i=1}^{n_p}\left\|\tilde{u}(\mathbf{x}^i) - u(\mathbf{x}^i)\right\|^2, \tag{4}$$

where $\mathbf{x}^i$ is the ith sample point and n_p is the total number of samples. Substituting $\boldsymbol{\beta}$ in Eq. (1), the PR metamodel is created.

2.2. Moving least squares

The Moving Least Squares method (MLS) was proposed by Lancaster in [10]. This approach uses the same logic as the polynomial regression but the coefficients $\boldsymbol{\beta}$ are functions of the spatial coordinates and they change from one point to another point. These coefficients can be determined if the number of sample points used for interpolation is equal to the number of coefficients. In MLS method, the unknown coefficients $\boldsymbol{\beta}$ are determined by minimizing the weighted least squares error $\mathrm{J}(\mathbf{x})$ [11]:

$$\mathrm{J}(\mathbf{x}) = \sum_{i=1}^{n_p} w_i(\mathbf{x})\|\mathbf{X}^T(\mathbf{x}^i)\boldsymbol{\beta}(\mathbf{x}) - u(\mathbf{x}^i)\|^2, \tag{5}$$

where $\mathbf{X}^T(\mathbf{x})$ is given according to Eq. (2). $w_i(\mathbf{x})$ is the weight function associated with the ith sample point. Different weight functions can be found in the literature (see [10,11,16]). One of the most common types is the *Gaussian* weight function of exponential type, which is given as:

$$w_i(\mathbf{x}) = e^{(-\|\mathbf{x}-\mathbf{x}^i\|^2/h^2)}, \tag{6}$$

where $\|\mathbf{x} - \mathbf{x}^i\|$ is the euclidean distance between the points $\mathbf{x}$ and $\mathbf{x}^i$ and parameter h is a constant value called spacing parameter. It should be mentioned here that the MLS method satisfies a condition in which the real function u and the approximation $\tilde{u}$ are equal at all n_p sample points.

2.3. POD-RBF

Proper Orthogonal Decomposition (POD) combined with Radial Basis Functions (RBF) is a recently developed method by Buljak [9]. POD-RBF finds the projection of the system response on a reduced space and then the approximation is carried out by using radial basis functions. The schematic flow-chart of POD-RBF method has been depicted in Fig. 1. The algorithm consists of two main parts (1) proper orthogonal decomposition of the snapshot matrix (2) interpolation using radial basis functions. The basic idea of proper orthogonal decomposition method is to present the snapshot matrix $\mathbf{U}$ as:

$$[\mathbf{U}]_{m\times n_p} = [\boldsymbol{\Phi}]_{m\times n_p}[\mathbf{A}]_{n_p\times n_p}, \tag{7}$$

here, $\mathbf{A}$ is the *amplitude matrix* and $\boldsymbol{\Phi}$ includes the *proper orthogonal basis vectors*. The POD basis vectors $\boldsymbol{\Phi}$ can be obtained by finding the normalized eigenvectors and eigenvalues of the symmetrical matrix $\mathbf{D} = \mathbf{U}^T\mathbf{U}$ (see [17]). Since the matrix $\boldsymbol{\Phi}$ fulfills the orthogonality condition i.e. $\boldsymbol{\Phi}^T = \boldsymbol{\Phi}^{-1}$, the amplitude matrix is calculated as follows:

$$[\mathbf{A}]_{n_p\times n_p} = \left[\boldsymbol{\Phi}^T\right]_{n_p\times m}[\mathbf{U}]_{m\times n_p}. \tag{8}$$

The size of matrix $\boldsymbol{\Phi}$ can be reduced if the basis vectors with small eigenvalues are omitted. To accomplish this, first the basis vectors are sorted in a descending order according to the magnitude of their eigenvalues. Then, the first k columns of matrix $\boldsymbol{\Phi}$ are taken and the rest are removed ($k \leqslant n_p$). In this way, the reduced basis vectors $\overline{\boldsymbol{\Phi}}^T$ can be obtained. Subsequently, the reduced amplitude matrix $\overline{\mathbf{A}}$ is calculated as follows:

$$\left[\overline{\mathbf{A}}\right]_{k\times n_p} = [\overline{\boldsymbol{\Phi}}^T]_{k\times m}[\mathbf{U}]_{m\times n_p}. \tag{9}$$

The second step is to use a linear combination of radially symmetric functions (Radial Basis Functions) in order to approximate the reduced amplitude matrix $\overline{\mathbf{A}}$. Having n_p sample points in the s dimensional space, each component of reduced amplitude matrix $\overline{\mathbf{A}}$ is computed by radial functions as follows:

$$\overline{a}_l^j = \sum_{i=1}^{n_p} b_l^i g_i(\mathbf{x}^j) \quad j = 1, \ldots, n_p \quad l = 1, \ldots, k, \tag{10}$$

where b_l^i are unknown coefficients and $g_i(\mathbf{x}^j)$ gives the value of the radial function g with the center point $\mathbf{x}^i$ at the sample point $\mathbf{x}^j$. Different types of radial functions have been proposed in the literature (see [7,11]). In this paper, *inverse multiquadratic* function is applied which has the form:

$$g_i(\mathbf{x}) = \left(\|\mathbf{x} - \mathbf{x}^i\|^2 + c^2\right)^{-0.5}, \tag{11}$$

where parameter c is a predefined constant which controls the smoothness of the radial basis function. It is computationally of advantage to select this value within the [0–1] range [9]. Fig. 2(a) and (b) shows two inverse multiquadratic radial basis functions with different values of c. With reducing the c parameter, the accuracy of POD-RBF metamodel might increase for nonlinear systems.

Eq. (10) provides $k \times n_p$ linear equations with $k \times n_p$ unknowns. This system of equations is solved to find the unknown coefficients.

$$\left[\overline{\mathbf{A}}\right]_{k\times n_p} = [\mathbf{B}]_{k\times n_p}[\mathbf{G}]_{n_p\times n_p} \Rightarrow [\mathbf{B}]_{k\times n_p} = \left[\overline{\mathbf{A}}\right]_{k\times n_p}[\mathbf{G}]^{-1}_{n_p\times n_p}, \tag{12}$$

here, matrix $\mathbf{G}$ gathers the values of radial functions at the sample points and matrix $\mathbf{B}$ includes the unknown coefficients. Finally, the equation below is used to find the function value at the observation point m for an arbitrary input point $\mathbf{x}$:

$$[\tilde{u}(\mathbf{x})]_{m\times 1} = \left[\overline{\boldsymbol{\Phi}}\right]_{m\times k}[\mathbf{B}]_{k\times n_p}[g_i(\mathbf{x})]_{n_p\times 1} \quad i = 1, \ldots, n_p. \tag{13}$$